Quantum Mechanics

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This note isn't intended for distribution. Quantum mechanics is discussed in detail. Links below show contents of solved problems and summary of special topics. Readers who have opened this note for the first time are highly recommended to read the preface.

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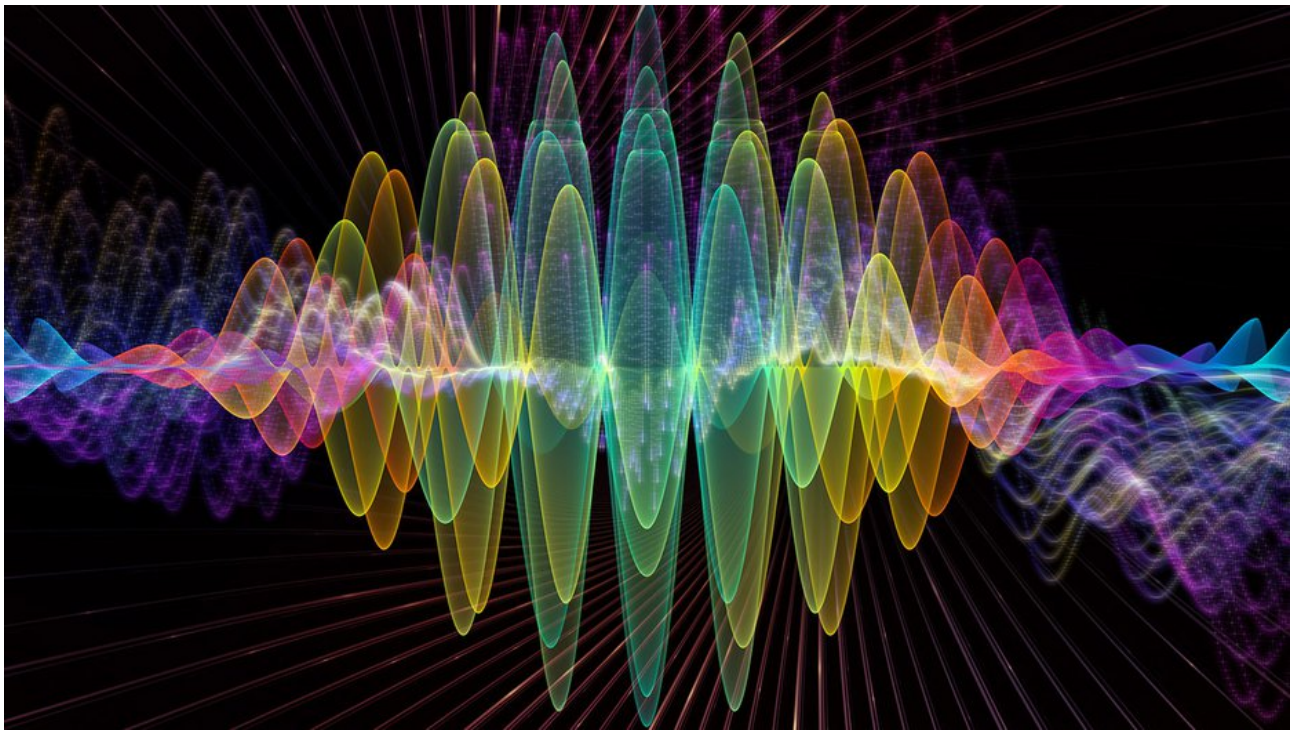
Preface, main motivation, main tips for studying



Overview of the note

Parts of the note are:
Fundamentals of Quantum Mechanics

Typical Methods and Models

Parts of Quantum Mechanics

Introduction to Other Parts of QM

The key sections are:
Perturbation Theories

Adiabatic methods

Semiclassical methods

Scattering theory: Fundamentals

Estimations and Features of Typical Models

This note contains special mathematical methods by Takhtajan, and approximate methods by Migdal, Krainov. I used the following literature.

(напишу потом качественно самое сильно мотивирующее, пока не готов писать, многие просто мотивирующие соображения - в дополнениях.)

Квантовая механика - один из самых основных предметов современной физики, без нее не следует вообще заниматься физикой, что бы человек ни делал

Да, я знаю, что можно сказать, что вот, мне по факту она не нужна, зачем ее учить? Потому что столько много предметов из нее идут! Столько много принципиально важных задач в рамках нее решаются. Да, пусть и методами, которые не обсуждаются в основном курсе квантмеха, но тем не менее. Уж слишком этот предмет важен для физики, чтобы какой-то физик мог заявить, что он профессионал, не владея основами квантмеха. К тому же, если человек умеет учиться, то это вообще не сложно.

(раскрою потом эту мысль)

Best general questions

m-ge.1 Как частица связана с волной? (!!!)

(так и не прописал четко ответ, потом пропишу)

(?? тут же про волны материи) (напряженность E, H....) и уравнения (формулы про волны) а с другой стороны: (???? формулы про частицы) Вопрос: как так получается и почему эти подходы эквивалентны?

(укажу потом ответ, пока обхожу стороной это.)

m-ge.2 Что такое измерение и как его описать?

m-ge.1 Что такое электрон?

(почему на это сложно отвечать? сформулирую свой ответ на этот вопрос)

m-ge.1 Почему атомы устойчивы?

(идейный ответ на этот вопрос именно квантовой механикой дается.)

m-ge.1 Описывая части системы, можно ли описать всю систему?

Оказывается, нет.
(тут пример Филиппова (?!!!))
(тут рассуждения и комментарии, мб еще пример приведу)

m-ge.1 Откуда берется спектр черного тела?

Best technical questions

(наберу самые лучшие - впишу, пока не уверен, какие они?)

m-te.1 I-motiv-1 Сколько будет спин параллелен полю?

Нейтрон находится в однородном магнитном поле $\mathcal{H}_0 \| z$. Определить время жизни состояния с проекцией спина на направление поля $m_s = +1/2$. Получить численное значение времени жизни для $\mathcal{H}_0 = 1$ кГс.

Указание к решению:
(напишу потом, пока в разделе с задачами это смотрю.)

m-te.2. Probability of ionization

Calculate the probability of ionization (removal of one electron from the atom) of a hydrogen atom when it collides with a neutron. Assume that momentum of neutron is given.

Указание к решению:
(напишу потом коротко суть решения, ЛЛ3 почитать нужно просто, чтобы разобраться.)
Answer:

$$W_{0k}dk = 2^8 \frac{v_{\text{n}}^2 \left(v_{\text{n}}^2 + \frac{1}{3}k^2 + \frac{1}{3}\right) e^{-\frac{2}{k}\,\text{arctg}\,\frac{2k}{v_{\text{n}}^2 - k^2 + 1}}}{\left[\left(v_{\text{n}} + k\right)^2 + 1\right]\left[\left(v_{\text{n}} - k\right)^2 + 1\right]\left[1 - e^{-2\pi/k}\right]} kdk.$$

m-te.3 (??) Что-то на момент и их сложение

Указание к решению:
(просто это типичная тема квантмеха, так что очень круто было бы это указать.)

Main tips for studying

В квантовой механике тупики в прогрессе понимания гораздо более вероятные, чем в других предметах, поэтому полезно указать особенности одного из правильных подходов к предмету.

Не занимайтесь долго вопросами о сути происходящего в квантмехе раньше времени и без повода

Очень важно забить на вопросы такого рода, потому что сил они кучу выедут, ничего не дадут. Итак полно заморочек, потом когда-то отвечу эти вопросы.

Не понимаешь волновую функцию? Ну и не важно, кто ее полностью понимает? Там вообще частица одновременно из всех координатных состояний в другое координатное состояние переходит. Это вообще не тот вопрос, которым следует заниматься, пока не прорешены задачи. И таких вопросов можно целую кучу задать.

Не циклитесь много на квантовой механике без потребности, нарешайте штук 100 задач, застабильте штук 15 ключевых тем и остальное уже по потребности доучивайте

Есть тысячи самых разных задач, большинство их, может, никто вообще не способен решить без отдельной подготовки к каждой. Они разные, разные темы есть. Не нужно требовать от себя знать всё или даже большинство тем. Так можно пару лет просто топтаться на месте, ничего в науке не достичь, деньги не заработать, ничего для мира не сделать.

Поэтому отдельно важно понимать, что пусть квантовая механика и базовый предмет, не нужно ставить целью пройти все её основы. Пара тем будет качественно отработана, минимальное количество задач будет нормально разобрано - всё, идем вперед и используем, доучиваем то, что требуется. И это абсолютно нормально не быть способным решить большинство задач, ибо альтернатива - ничего не сделать в жизни, но только набивать руку в том, что скорее всего не будет использоваться.

Конечно, важно понимать и другую мысль, что действительно нужно минимальные основы хорошо понять и если они не усвоены и если есть возможность - действительно, следует их доработать. Просто не об этом речь сейчас.

Не ведитесь на тех, кто предлагает курсы по квантовой механике, если уже прошли другой нормальный курс и нет потребности в рамках актуального проекта в ней! Такие

предложения - это предложения потоптаться на месте. Разве что если это не мировой авторитетный ученый в области квантовой механики, но даже в таком случае скорее всего правильнее отказаться от таких доп. курсов, потому что опять же, предмет большой, даже все основы изучать - слишком большое и редко применяющееся дело.

Следуйте структурному подходу

Конечно, я всегда в рамках него и работаю, но именно на квантовой механике становится понятно, что без структур начинается огромная путаница. Другие же предметы могут взяться и без структур, а вот квантовая механика в ее современной форме скорее всего в принципе не возьмется. Слишком много разных теорией, разных вопросов, разных задач, просто не вырулить, если без структур работать.

Part I
Typical Quantum Mechanics in a Nutshell

1 Main laws, methods, models

1.1 Main laws and properties of QM

1.1.1 Schrodinger, Heisenberg equations, wave function

Суть уравнения Шредингера

non-stationary: $i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi,$ $\hat{H} = i\hbar\frac{\partial}{\partial t}$

stationary: $\hat{H}\left|\psi_E\right\rangle = E\left|\psi_E\right\rangle.$ e.v. of H

non-stationary: $\left|\psi_E(t)\right\rangle = \sum_n \left|n\right\rangle e^{-iE_nt/\hbar}\langle n|\psi\rangle$

stationary: $\left|\psi(t)\right\rangle = \hat{U}(t)\left|\psi_E\right\rangle \equiv e^{-i\hat{H}t/\hbar}\left|\psi_E\right\rangle = e^{-iEt/\hbar}\left|\psi_E\right\rangle$

Если задача на стационарное состояние в 1D потенциале:

1/4) Пишем уравнение Шредингера $\psi'' + \frac{2m}{\hbar^2}(E - U(x))\psi(x) = 0$; если потенциал в виде "ступенек", то пишем систему для каждой зоны.

2/4) Вводим обозначения для констант, пишем предполагаемый вид волновой функции, через сумму экспонент или гармоник.

3/4) Сшиваем по равенству логарифмичекой производной $\psi'/\psi|_1 = \psi'/\psi|_2$, получаем уравнение или систему уравнений, из нее - уровни энергии.

4/4) Доходим до ответа (??? как???)

Probability of changing the state is

$$P = \langle\psi_2|\psi_1\rangle.$$

Thus we often evaluate coefficient in front of the wavefunction and it gives the probability of changing the state. The probability of staying in the same state can be found also by subtraction from one the probability of change.

Важно следовать этому алгоритму и не скакать, потому что иначе можно запутаться, какие параметры когда появились и что требуется искать!

(?? а в импульсном предст когда удобнее???)

(тут очень коротко про задачи, вообще ниже в моделях все указания)

Свойства и частные случаи уравнения Шредингера

Типичные свойства Уравнения Шредингера

$$\psi(x) \approx \begin{cases} a_L e^{ikx} + b_L e^{-ikx}, & x \to -\infty \\ a_R e^{ikx} + b_R e^{-ikx}, & x \to +\infty \end{cases}$$

(допишу потом, в контексте задач на это)

$$\psi_k^{(+)}(x) = \begin{cases} e^{ikx} + re^{-ikx}, & x \to -\infty \\ te^{ikx}, & x \to +\infty \end{cases}, \qquad \psi_k^{(-)}(x) = \begin{cases} t'e^{-ikx}, & x \to -\infty \\ e^{-ikx} + r'e^{ikx}, & x \to +\infty \end{cases}$$

$$\begin{cases} t' &= t \\ r' &= -r^* t/t^* \end{cases} \qquad \text{(time rev sym)}$$

Об уравнении Шредингера в импульсном представлении (!?!?!??!?!?)

$$\frac{\boldsymbol{p}^2}{2m}\psi(\boldsymbol{p}) + \int \frac{d^D\boldsymbol{p}}{(2\pi)^d}\psi(\boldsymbol{p}')\, U_{\boldsymbol{p}-\boldsymbol{p}'} = E\psi(\boldsymbol{p})$$

Для перехода полезны формулы преобразования Фурье.
(напишу тут их.)

$$\langle p|U(\hat{x})|p'\rangle = \left\langle p\left|U(\hat{x})\int dx\right|x\right\rangle\langle x|p'\rangle = \int dx U(x)\langle p|x\rangle\langle x|p'\rangle = \int dx U(x)e^{-i(p-p')x} = U_{p-p'}$$

$$\langle \boldsymbol{p}|U(\hat{\boldsymbol{x}})|\psi\rangle = \langle \boldsymbol{p}|U(\hat{\boldsymbol{x}})\underbrace{\int (d\boldsymbol{p}')\,|\boldsymbol{p}'\rangle\langle\boldsymbol{p}'|}_{\hat{\mathbb{I}}}(d\boldsymbol{p}')\, U_{\boldsymbol{p}-\boldsymbol{p}'}\psi(\boldsymbol{p}')$$

$(d\boldsymbol{p}) \equiv d^d\boldsymbol{p}/(2\pi)^d$.

Useful approximations:

$$\int_0^\infty \left(\frac{\exp(-ku)}{\sqrt{1+u^2}}\right)du \approx \int_0^{1/k}\frac{du}{\sqrt{1+u^2}} = \ln\left[u+\sqrt{1+u^2}\right]\Big|_0^{1/k} = \ln\left(\frac{2}{k}\right)$$

(!! другие приближения напишу!)

(!?!?!? абзац про смысл происходящего, и почему так можно вообще делать?)

Дальше можно точно решать (????? я хз, там сумма функций часто от разных аргументов, я такое решать не умею.)
Но часто решаем приближенно.

О стационарных состояниях

Связь представления Шредингера и других представлений (???)

потом пропишу, я кстати хз, зачем оно нужно.
В Гейзенберга:
(????)
в представление взаимодействия:
(???)
на деле ни разу не использовал пока что

О выводе УШ

(тоже полезно помнить)

О влиянии геометрии на квантовую динамику (???)

(частица там вылетит из сопла, треугольник, эллипс, в чем особенности таких задач?? пропишу потом)

Энергия поперечного движения оценивается как

$$\varepsilon^{(f)}(z) \sim \frac{1}{mR^2(z)},$$

ибо $\varepsilon = \frac{1}{2m}\frac{\partial^2}{\partial^2 x}$.

(!! порешаю - пропишу.)

О неортонормированном базисе (???)

Если базисные вектора не являются ортогональными, нужно вычислить матрицу Грама для этого базиса (это матрица скалярных произведений $G_{ij} = \langle\psi_i|\psi_j\rangle$).

Характеристическое уравнение, определяющее собственные числа для неортонормированного базиса, имеет вид $\det(\hat{H} - E \cdot \hat{G}) = 0$. Найдите собственные уровни энергии в заданном приближении.

(см. задачу пока, такое пока только раз нужно было, но потом еще попрактикуюсь. крутой очень метод!)

Преобразования уравнения Шредингера в другие координаты и для решений через спецфункции

(???? из ЛЛ3 многое добавлю про это!)

В сферических

$$\Delta\phi = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\phi$$

В цилиндрических

$$-\frac{\hbar^2}{2M}\left(\frac{\partial^2\psi}{\partial r^2} + \frac{1}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\varphi^2}\right) + U(r)\psi(r) = E\psi(r)$$

$$\psi(r,\varphi) \equiv \psi(r)e^{im\varphi} \qquad \psi''(r) + \frac{1}{r}\psi'(r) - \left(\frac{2MU(r)}{\hbar^2} + x^2 + \frac{m^2}{r^2}\right)\psi(r) = 0$$

Для связных состояний ($E < 0$), ответ, учитывающий $\psi(r \to \infty) \to 0$:

$$\psi(r > a) = AK_m(\varkappa r).$$

А в общем случае:

$$\psi(z) = A_1 I_m(z) + A_2 K_m(z)$$

$$z \gg 1 \qquad I_m(z) \approx \frac{1}{\sqrt{2\pi z}} e^z, \qquad K_m(z) \approx \sqrt{\frac{\pi}{2z}} e^{-z},$$
$$z \ll 1 \qquad I_m(z) \approx \frac{1}{m!}\left(\frac{z}{2}\right)^m, \qquad K_m(z) \approx \begin{cases} \frac{(m-1)!}{2}\left(\frac{2}{z}\right)^m, & m \neq 0 \\ \ln\frac{2}{z} - \gamma, & m = 0 \end{cases}$$

О решении через гипергеометрическую функцию ${}_2F_1(a,b;c;x)$ (!??!?!?)

$$z(1-z)f''(z) + (c-(a+b+1)z)f'(z) - abf(z) = 0, \qquad c \neq 1,\ f(0) = 1,$$
$$f(z) = C_1 {}_2F_1(a,b;c;z) + C_2 z^{1-c} {}_2F_1(b-c+1, a-c+1; 2-c; z),$$

где

(?? укажу, что это за функции тут!)

Метод применяется в задачах релятивисткой квантовой механики и скорее всего в других темах.

(какие-то основные свойства гип геом ф-ции тут для полноты добавлю)

О решении через вырожденную гипергеометрическую функцию ${}_1F_1(a,b;x)$ (!??!?!?)

$$zf''(z) + (b-z)f'(z) - af(z) = 0, \quad f(0) = 1,$$
$$f^{(2)}(z) = z^{1-b} {}_1F_1(a-b+1; 2-b; z).$$

(?? укажу, что это за функции тут!)

Например, для осциллятора именно этот метод работает!

(пока тоже не много нарешал такого еще)

волновой функции

Определение и основные свойства волновой функции

(важный абзац со смыслом ее!)

$$\int_V \Psi^* \Psi dv = 1$$

(важный абзац про то, откуда это появилось????)

Среднее наблюдаемой q:

$$\langle q \rangle = \sum_{\{q\}} q|\Psi(q)|^2 \equiv \sum_{\{q\}} q\Psi^*(q)\Psi(q) \equiv \sum_{\{q\}} q\langle\Psi|q\rangle\langle q|\Psi\rangle$$

Введем для наблюдаемой $\{q\}$ оператор $\hat{Q}$ такой, что

$$\hat{Q}|q\rangle = q|q\rangle$$

Отсюда (????) $\langle q \rangle = \sum_{\{q\}} \langle\Psi|Qq\rangle\langle q|\Psi\rangle$ и $\langle q \rangle = \langle\Psi|Q\Psi\rangle$.

(тут про то, как это было бы, если бы были открытые сист и запутанность?)

Волновые функции могут быть нормируемые на дельта-функцию, например, это так для свободной частицы в пустоте. (? а что с в.ф. в магнитном поле, уровни Ландау насколько меняют нормировку?)

Связь волновой функции с другими квантовым параметрами (!!)

энергия
матрица плотности
ток
связь волновой функции фотона ψ и напряженности поля волны $\vec{E}$
(?!!!)

О смысле и интерпретациях волновой функции и ее коллапса (??)

(тут суть этого напишу, что есть, какой смысл? подробно - раздел далеко внизу)

потоке вероятности и уравнении непрерывности (?!)

$$\begin{aligned} j(x) &= \operatorname{Re}\psi^*\hat{v}\psi \equiv \\ &\equiv -\frac{i\hbar}{2m}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) \equiv \\ &\equiv \frac{\hbar}{m}|\psi(\boldsymbol{r})|^2\nabla\varphi \qquad\qquad \psi(\boldsymbol{r}) \equiv |\psi(\boldsymbol{r})|e^{i\varphi(\boldsymbol{r})}. \end{aligned}$$

$$\frac{\partial}{\partial t}\rho(\boldsymbol{r},t) = \frac{\partial}{\partial t}\left\{\Psi^*(\boldsymbol{r},t)\Psi(\boldsymbol{r},t)\right\} = \tfrac{\mathrm{i}}{\hbar}\left\{(\hat{H}\Psi^*)\Psi - \Psi^*(\hat{H}\Psi)\right\} \equiv -\boldsymbol{\nabla}\cdot\boldsymbol{j} \qquad \Rightarrow$$

$$\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{j} = 0.$$

$$\int\limits_V d^2r\,\mathrm{div}\,j = \oint\limits_{\partial V} j\cdot ds = 0$$

Поток вероятности через поверхность, в которой находится квантовая частица, должен быть равен нулю.

(!!! не раскрыто, как пользоваться j????? пока не знаю, ну есть это, ну и все на том... напишу потом. по идее эти формулы и используем для задач о вероятности перехода.)

О волновом пакете (???)

$$\Psi(\boldsymbol{r},t) \equiv \int \frac{d^3p}{(2\pi\hbar)^3}\tilde{\Psi}(\boldsymbol{p})e^{\frac{\mathrm{i}}{\hbar}(\boldsymbol{p}\cdot\boldsymbol{r}-Et)}$$

(??)

Proof:

$$\Psi(\boldsymbol{r},t) = \langle\boldsymbol{r}|\Psi(t)\rangle = \int\langle\boldsymbol{r}|\boldsymbol{p}\rangle\frac{d^3p}{(2\pi\hbar)^3}\langle\boldsymbol{p}|\Psi(t)\rangle$$

где (????)

$$\langle\boldsymbol{r}|\boldsymbol{p}\rangle = \Psi_{\boldsymbol{p}}(\boldsymbol{r}) = e^{\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}, \quad \langle\boldsymbol{p}|\Psi(t)\rangle = e^{-\frac{1}{\hbar}Et}\langle\boldsymbol{p}|\Psi\rangle = e^{-\frac{1}{\hbar}Et}\tilde{\Psi}(p)$$

Для движения фронта волны: $\phi = \mathrm{const}$,

$$\boldsymbol{r}(t) = \frac{E}{p^2}\boldsymbol{p}t + \boldsymbol{r}_0 \quad \rightarrow \quad \phi = \boldsymbol{p}\cdot\boldsymbol{r}_0 + \hbar\alpha(\boldsymbol{p}) = \ \mathrm{const}.$$

$$\boldsymbol{v}_{\text{ph}} := \frac{E}{p^2}\boldsymbol{p}$$

(????)

размерностях и оценках в квантовой механике (!!!)

(тут крутые методы, скоро пропишу!)

Уравнение Гейзенберга

(мб потом напишу, пока повесит пусть, ну или удалю.)

1.1.2 Axioms of QM, measurements

(По Тахтаджаяну. Не до этого, не хочу этим заниматься, сперва уровень теормина.)

Аксиомы квантовой механики Дирака-фон Неймана. (тут же аксиома об измерении)

1. A1. С любой квантовой системой ассоциировано бесконечномерное сепарабельное комплексное гильбертово пространство $\mathscr{H}$. (В физической терминологии оно называется пространством чистых состояний.) Гильбертово пространство составной квантовой системы - это тензорное произведение гильбертовых пространств компонент системы.

2. A2. Множество наблюдаемых $\mathscr{A}$ квантовой системы $\mathscr{H}$ - это все самосопряженные операторы в $\mathscr{H}$. Подмножество $\mathscr{A}_0 = \mathscr{A} \cap \mathscr{L}(\mathscr{H})$ ограниченых наблюдаемых является векторным пространством над $\mathbb{R}$.

3. A3. Множество состояний $\mathscr{S}$ квантовой системы с гильбертовым пространством $\mathscr{H}$ состоит из всех положительных (а значит, самосопряженных) операторов M со следом $\operatorname{Tr} M = 1$. Чистые состояния это операторы проектирования (проекторы) на одномерные подпространства $\mathscr{H}$.

   Для $\psi \in \mathscr{H}, \|\psi\| = 1$, соответствующий проектор на $\mathbb{C}\psi$ обозначается P_ψ. Все остальные состояния называются смешанными состояниями.

4. A4. Процесс измерения - это сопоставление каждой наблюдаемой $A \in \mathscr{A}$ и состоянию $M \in \mathscr{S}$ вероятностную меру μ_A на $\mathbb{R}$:

   $$\mathscr{A} \times \mathscr{S} \ni (A, M) \mapsto \mu_A \in \mathscr{P}(\mathbb{R}),$$

   и она - это вероятность того, что для квантовой системы в состоянии M результат измерения наблюдаемой A принадлежит E, $E \subseteq \mathbb{R}$ - любое борелевское подмножество. То есть она в пределах: $0 \leqslant \mu_A(E) \leqslant 1$. Конкретно, для нее есть формула Борна-фон Нейиана:

   $$\mu_A(E) = \operatorname{Tr} \mathrm{P}_A(E)M, \quad E \in \mathscr{B}(\mathbb{R})$$

   Математическое ожидание (среднее значение) наблюдаемой $A \in \mathscr{A}$ в состоянии $M \in \mathscr{S}$ - это

   $$\langle A|M\rangle = \int_{-\infty}^{\infty} \lambda d\mu_A(\lambda)$$

$\mu_A(\lambda) = \mu_A((-\infty, \lambda))$ - функция распределения вероятностной меры μ_A. (???? непонятно, что значит этот интеграл???)

(???? я пока не вижу, почему именно такие аксиомы нужным нам и как они проявляются. Потом додумаю.)

(???? есть много про это теории в записи про квантовую теорию информации, там в первую очередь буду её разбирать и прописывать)

О состояниях, мерах, определениях операторов

Состояние $M \in \mathscr{S}$ - чистое, если и только если его нельзя представить в виде нетривиальной линейной комбинации в $\mathscr{S}$.

Определение. Проекторная мера на $\mathbb{R}$ - это отображение P: $\mathscr{B}(\mathbb{R}) \to \to \mathscr{L}(\mathscr{H})\sigma$-алгебры $\mathscr{B}(\mathbb{R})$ борелевских подмножеств $\mathbb{R}$ в алгебру ограниченных операторов в $\mathscr{H}$, удовлетворяющее следующим свойствам.

PM1. Для любого борелевского подмножества $E \subseteq \mathbb{R}$, оператор $\mathrm{P}(E)$ ортогональная проекция, т. е. $\mathrm{P}(E) = \mathrm{P}(E)^2$ и $\mathrm{P}(E) = \mathrm{P}(E)^*$.

PM2. $\mathrm{P}(\emptyset) = 0, \mathrm{P}(\mathbb{R}) = I$, единичный оператор в $\mathscr{H}$.

PM3 Для любого дизъюнктного объединения борелевских подмножеств

$$E. = \coprod_{n=1}^{\infty} E_n, \quad \mathrm{P}(E) = \lim_{n\to\infty} \sum_{i=1}^{n} \mathrm{P}\left(E_i\right)$$

в сильной топологии $\mathscr{L}(\mathscr{H})$.

С любой проекторной мерой P на $\mathbb{R}$ ассоциируется проекторнозначная функция

$$\mathrm{P}(\lambda) = \mathrm{P}((-\infty, \lambda)),$$

называемая проекторным разложением единицы. Она характеризуется следующими свойствами. PD1.

$$\mathrm{P}(\lambda)\mathrm{P}(\mu) = \mathrm{P}(\min\{\lambda, \mu\}).$$

PD2.

$$\lim_{\lambda\to-\infty} \mathrm{P}(\lambda) = 0, \lim_{\lambda\to\infty} \mathrm{P}(\lambda) = I.$$

PD3.

$$\lim_{\substack{\mu\to\lambda \\ \mu<\lambda}} \mathrm{P}(\mu) = \mathrm{P}(\lambda)$$

Измеримая функция f на $\mathbb{R}$ называется финитной почти везде (п. в.) по отношению к проекторной мере P, если она финитна п. в. по отношению ко всем мерам $(\mathrm{P}\psi, \psi), \psi \in \mathscr{H}$. Для сепарабельного $\mathscr{H}$ теорема фон Неймана утверждает, что для любой проекторной меры P существует $\varphi \in \mathscr{H}$, такое, что функция f финитна п. в. по отношению к P, если и только если она финитна п. в. по отношению к мере $(\mathrm{P}\varphi, \varphi)$.

Теорема Дж. фон Неймана по Тахтаджаяну. Для любого самосопряженного оператора A в гильбертовом пространстве $\mathscr{H}$ существует единственое проекторное разложение единицы $\mathrm{P}(\lambda)$, удовлетворяющее следующим свойствам.

(i)

$$D(A) = \left\{ \varphi \in \mathscr{H} : \int_{-\infty}^{\infty} \lambda^2 d(\mathrm{P}(\lambda)\varphi, \varphi) < \infty \right\},$$

и для любого $\varphi \in D(A)$

$$A\varphi = \int_{-\infty}^{\infty} \lambda d\mathrm{P}(\lambda)\varphi$$

определенный как предел сумм Римана-Стильтьеса в сильной топологии на $\mathscr{H}$. Носитель соответствующей проекторной меры P совпадает со спектром оператора A : $\lambda \in \sigma(A)$, если и только если $\mathrm{P}'_A((\lambda-\varepsilon, \lambda+\varepsilon)) \neq 0$ для любого $\varepsilon > 0$.

(ii) $\forall f \in C[\mathbb{R}]$, $f(A)$: $D(f(A)) = \left\{\varphi \in \mathscr{H} : \int_{-\infty}^{\infty} |f(\lambda)|^2 d(\mathrm{P}(\lambda)\varphi, \varphi) < \infty\right\}$, $\forall \varphi \in D(f(A))$

$$f(A)\varphi = \int_{-\infty}^{\infty} f(\lambda) d\mathrm{P}(\lambda)\varphi$$

и понимаемый, как в части (i).

$$f(A)^* = \bar{f}(A)$$

$\bar{f}$ - комплексно сопряженная функция κf, а оператор $f(A)$ ограничен, если и только если функция f ограничена на $\sigma(A)$. Для ограниченных на $\sigma(A)$ непрерывных функций f u g

$$f(A)g(A)\varphi = \int_{-\infty}^{\infty} f(\lambda)g(\lambda) d\mathrm{P}(\lambda)\varphi, \quad \varphi \in \mathscr{H}$$

(iii) Для любой измеримой функции f на $\mathbb{R}$, конечной п. в. по отночению κ проекторной мере $\mathrm{P}, f(A)$ - линейный оператор в $\mathscr{H}$, определенный, как в (ii), где интеграл для $f(A)\varphi$ теперь понимается в слабом смысле: для $\varphi \in D(f(A))$ и любого $\psi \in \mathscr{H}$

$$(f(A)\varphi, \psi) = \int_{-\infty}^{\infty} f(\lambda) d(\mathrm{P}(\lambda)\varphi, \psi)$$

- интеграл Лебега-Стильтьеса по отношению к комплексной мере. Соответствие $f \mapsto f(A)$ удовлетворяет тем же свойствам, что и в (ii), где интегралы понимаются в слабом смысле.

(iv) Ограниченный оператор B коммутирует с A, то есть $B(D(A)) \subset \subset D(A)$ и $AB = BA$ на $D(A)$, если и только если он коммутирует с $\mathrm{P}(\lambda)$ для всех λ, и, следовательно, B коммутирует с любьи оператором $f(A)$.

(v) Для любого проекторного разложения единицы $\mathrm{P}(\lambda)$ оператор A в $\mathscr{H}$, определенный, как в части (i), самосопряжен.

Canonical quantization

Квантование классических систем каноническим образом происходит за счет замены скобки пуассона переходит на коммутатор:

$$\{q, p\}_{\mathrm{P}} = 1 \quad \longrightarrow \quad [\hat{q}, \hat{p}] = \mathrm{i}\hbar$$

Покажем это.

(короче, я не уверен, как это сделать, тут пока накидывание)

Производная по времени имеет вид:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \left\{\frac{\partial f}{\partial q}\dot{q} + \frac{\partial f}{\partial p}\dot{p}\right\}$$

$$df = \frac{\partial f}{\partial q}dq + \frac{\partial f}{\partial p}dp = 0$$

Тогда дифференциал g можно записать через дифференциал f:

$$dg = \frac{\partial g}{\partial q}dq + \frac{\partial g}{\partial p}dp = dq\left\{\frac{\partial g}{\partial q}\frac{\partial f}{\partial p} - \frac{\partial g}{\partial p}\frac{\partial f}{\partial q}\right\}\frac{1}{\partial f/\partial p}$$

$$dg = dq\{g,f\}_{\mathrm{P}}\frac{1}{\partial f/\partial p}$$

$$\delta g\delta f \simeq \{g,f\}_{\mathrm{P}}\delta q\delta p$$

$$\delta g\delta f \simeq \{g,f\}_{\mathrm{P}}\Delta\Gamma$$

$$\Delta g\Delta f \simeq |[\hat{g},\hat{f}]|$$

$$[\hat{f},\hat{g}] = \{f,g\}_{\mathrm{P}}\cdot \mathrm{i}\hbar$$

кстати, уравнение Гейзенберга тут тоже относится к этому.

$$\mathrm{i}\hbar\frac{d\hat{f}}{dt} = \mathrm{i}\hbar\frac{\partial\hat{f}}{\partial t} + [\hat{f},\hat{H}]$$

Примеры

вторичном квантовании

(очень важная тема, напишу скоро, пока в КТП, конд средах или еще где-то.)

Основные методы и формулы вторичного квантования

Примеры вторичного квантования

проективных измерениях (????)

(??? путаюсь, заново учить нужно!)

смешанности состояний и других основах (????)

(заготовка основ для кв теор инф, в ней уже они применяться будут)

О типичных заблуждениях про измерения

О гамильтонианах в квантовой механике

зависимость гамильтониана от параметра теорема Гельмана — Фейнмана:

$$\frac{\partial E_n(\lambda)}{\partial\lambda} = \int \Psi_n^*(\lambda)\frac{\partial \mathrm{H}(\lambda)}{\partial\lambda}\Psi_n(\lambda)d\tau$$

(тут строчка про применения ее (?????))

(тут формулы преобразования Гамильтониана при переходе в новую СК в случаях, если он зависит от времени или не зависит.)

(??? о неэрмитовых гамильтонианах, откуда они вообще могут взяться??? открытые системы, так просто??)

Об операторе эволюции

(самое основное про него пока тут)

$$|\psi(t)\rangle = \hat{U}(t)|\psi\rangle$$

$$\hat{U}(t) = \lim_{N\to\infty}\prod_{k=1}^{N}\hat{\mathrm{T}}\left\{e^{-\frac{\mathrm{i}}{\hbar}\hat{H}(t_k)dt}\right\} = \hat{\mathrm{T}}\left\{e^{-\int\frac{1}{\hbar}\hat{H}(t)dt}\right\},$$

$$\hat{U}(t) = \exp(-i\hat{H}t/\hbar), \qquad H \neq H(t).$$

случай дискретного спектра

(сперва методы работы с ним, потом - примеры именно моделей с ним)

способе измерений (????)

(??? пока хз, еще не уверен в ответах на это.)
(это вечный вопрос, пока не хочу на это тратить время)
(просто указания на все ответы про них, как раз 1 раздел и нужен, пока не особо думал про это)

Типичные явления с измерениями

О квантовом парадоксе Зенона

(??? впишу, как описать его?? пока см. задачу про 2х уровневую систему, там пока решил это.)

Что может быть, а чего не может быть во время измерений?

(очень много идейно важных вопросов, поэтому их тут сразу и указываю! всё это с профессионалами нужно обсуждать.)

Может ли после измерения частица остаться в том же состоянии, в котором и была до измеренеия?

другом про измерения

О принципе суперпозиции состояний

(упомянуть все-таки стоит того, но особо много писать не вижу пока смысла, когда-то потом гораздо подробнее изучу - мб тогда больше укажу тут.)

1.1.3 Quantum operators, angular momentum

Определения основных операторов и их смысл

О типичных квантовых операторах и их свойствах

$$\hat{p}\psi(x) = -i\hbar\frac{\partial\psi}{\partial x}$$

$$[x, P] = i\hbar$$

$$\hat{T}_a = e^{a\frac{\partial}{\partial x}}$$

$$\hat{T}_a|x\rangle \underset{\text{def.}}{\equiv} |x-a\rangle.$$

$$\hat{T}_a\psi(x) \underset{\text{def.}}{\equiv} \langle x|\hat{T}_a|\psi\rangle = \langle \hat{T}_a^\dagger x|\psi\rangle = \langle x+a|\psi\rangle = \psi(x+a).$$

Momentum operator in spherical coordinates

О задачах на оператор момента импульса (?)

(тоже специфика есть.)

Алгоритм вывода вида операторов

(там что-то из ур Гейзенберга получать нужно, напишу потом, есть на это задачи)
(абзац про оператор времени, там статья есть, крутая идея, но нужно подумать минимум полчаса про это. Мб еще день тренироваться в этой идеи, пробовать применять его. пока не актуально.)

Об угловом моменте

Для $H = \frac{\boldsymbol{P}^2}{2m} + V(\boldsymbol{Q})$ со сферическим $V(\boldsymbol{x}) = V(|\boldsymbol{x}|)$ операторы M_1, M_2, M_3 и M^2, - квантовые интегралы движения:

$$[H, M_1] = [H, M_2] = [H, M_3] = 0; \qquad \left[H, M^2\right] = 0. \quad \text{(integrals)}$$

$$\{M_j, P_k\}_\hbar = -\varepsilon_{jkl}P_l, \quad \{M_j, Q_k\}_\hbar = -\varepsilon_{jkl}Q_l, \quad j,k,l = 1,2,3,$$

$$M_1 = i\hbar\left(x_3\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_3}\right), \quad M_2 = i\hbar\left(x_1\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_1}\right), \quad M_3 = i\hbar\left(x_2\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_2}\right).$$

$$\forall\psi:\ \psi(\boldsymbol{x}) = \psi(|\boldsymbol{x}|). \qquad M_1\psi = M_2\psi = M_3\psi = 0$$

$$x_1 = r\sin\vartheta\cos\varphi, \quad x_2 = r\sin\vartheta\sin\varphi, \quad x_3 = r\cos\vartheta,$$

$0 \leqslant \vartheta < \pi, 0 \leqslant \varphi < 2\pi$

$$M_1 = i\hbar\left(\sin\varphi\frac{\partial}{\partial\vartheta} + \cot\vartheta\cos\varphi\frac{\partial}{\partial\varphi}\right), \quad M_2 = -i\hbar\left(\cos\varphi\frac{\partial}{\partial\vartheta} - \cot\vartheta\sin\varphi\frac{\partial}{\partial\varphi}\right), \quad M_3 = -i\hbar\frac{\partial}{\partial\varphi}.$$

$$\boldsymbol{M}^2 = -\hbar^2\left(\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right),$$

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}\boldsymbol{M}^2$$

$$\hat{p}_r = \frac{1}{2}\left(\frac{\boldsymbol{r}}{|\hat{\boldsymbol{r}}|}\cdot\hat{\boldsymbol{p}} + \hat{\boldsymbol{p}}\cdot\frac{\boldsymbol{r}}{|\hat{\boldsymbol{r}}|}\right), \qquad \text{(Hermitian)}$$

$$\boldsymbol{p}^2\psi(\boldsymbol{r}) = \left({p_r}^2 + \frac{\boldsymbol{L}^2}{r^2}\right)\psi(\boldsymbol{r})$$

$$\hat{\boldsymbol{L}}^2 = \hat{\boldsymbol{r}}^2\hat{\boldsymbol{p}}^2 - (\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}})^2 + i\hbar\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}}$$

$$p_r = \frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r}r, \qquad p_r^2 = -\hbar^2\frac{1}{r}\frac{\partial^2}{\partial r^2}r, \qquad \frac{\boldsymbol{L}^2}{\hbar^2} = -r^2\nabla^2 + \frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) = -r^2\nabla^2 - \frac{r^2}{\hbar^2}p_r^2,$$

$$[p_r, r] = -i\hbar, \qquad \left[p_r, r^2\right] = -2i\hbar r, \qquad [p_r, r^n] = -ni\hbar r^{n-1},$$

$$\left[r, p_r^2\right] = 2i\hbar p_r, \qquad \left[r, p_r^3\right] = 3i\hbar p_r^2, \qquad \left[p_r, \frac{1}{r}\right] = \frac{i\hbar}{r^2}$$

$$\left[p_r, \frac{1}{r^2}\right] = \frac{2i\hbar}{r^3} \qquad \left[p_r^2, \frac{1}{r^2}\right] = -\frac{2\hbar^2}{r^4}\left(1 - 2r\frac{\partial}{\partial r}\right), \qquad \left[p_r^2, \frac{1}{r}\right] = \frac{2\hbar^2}{r^2}\frac{\partial}{\partial r}$$

$$p_x = \cos\phi p_r - \frac{\sin\phi}{r}p_\phi,$$

$$p_y = \sin\phi p_r + \frac{\cos\phi}{r}p_\phi.$$

О представлениях SO(3)

Группа вращений SO(3) - группы ортогональных матриц 3×3 с определителем 1. Она компактная группа Ли, изоморфная вещественному проективному пространству $\mathbb{RP}^3$ как гладкое многообразие. Имеется изоморфизм групп Ли $\mathrm{SO}(3) \simeq \mathrm{SU}(2)/\{\pm I\}$, SU(2) - группа Ли унитарных матриц 2×2 с определителем 1. Алгебра Ли $\mathfrak{so}(3)$ группы SO(3) - трехмерная алгебра Ли кососимметрических матриц 3×3 с базисом

$$X_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad X_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad X_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

$$[X_1, X_2] = X_3, \qquad [X_2, X_3] = X_1, \qquad [X_3, X_1] = X_2$$

Матрицы X_1, X_2, X_3 порождают соответственно однопараметрические подгруппы SO(3), состоящие из вращений вокруг координатных осей в $\mathbb{R}^3$.

Чтобы установить связь между квантовыми операторами углового момента и теорией представлений SO(3), рассмотрим регулярное представление R группы SO(3) в $\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{x})$, определенное формулой

$$(R(g)\psi)(\boldsymbol{x}) = \psi\left(g^{-1}\boldsymbol{x}\right), \quad g \in \mathrm{SO}(3), \psi \in \mathscr{H}$$

Лемма 3.1. Имеем

$$R\left(e^{u_1X_1+u_2X_2+u_3X_3}\right) = e^{-\frac{i}{\hbar}(u_1M_1+u_2M_2+u_3M_3)}$$

Все неприводимые унитарные представления R_l группы Ли SO(3) конечномерны и параметризуются неотрицательными целыми числами $l \geqslant 0$. Соответствующее неприводимое представление $\rho_l = dR_l$ алгебры Ли so(3) в $2l+1$-мерном комплексном векторном пространстве V_l можно явно описать следующим образом. Введем эрмитовы операторы $T_j = i\rho_l(X_j)$, $j = 1, 2, 3$, удовлетворяющие коммутационным соотношениям

$$[T_1, T_2] = iT_3, \quad [T_3, T_1] = iT_2, \quad [T_2, T_3] = iT_1$$

В векторном пространстве V_l есть ортонормированный базис $\{e_{lm}\}_{m=-l}^{m=l}$, такой, что

$$\begin{aligned}(T_1 - iT_2)\, e_{lm} &= -\sqrt{(l+m)(l-m+1)}e_{lm-1},\\ (T_1 + iT_2)\, e_{lm} &= -\sqrt{(l-m)(l+m+1)}e_{lm+1},\\ T_3 e_{lm} &= m e_{lm}.\end{aligned}$$

В частности, $(T_1 + iT_2)\, e_{ll} = 0$, так что V_l - модуль со старшим весом. Представление ρ_l неприводимо, и по лемме Шура

$$\boldsymbol{T}^2 = l(l+1)I_l,$$

I_l - тождественный оператор в V_l. Это можно также прямо проверить, используя (3.10) - (3.12).

Когда l - полуцелое число, т.е. $l \in \frac{1}{2} + \mathbb{Z}_{\geqslant 0}$, и $m = -l, -l+1, ..., l-1, l$, формулы (3.10) - (3.12) все еще определяют неприводимое представление ρ_l старшего веса алгебры Ли $\mathfrak{so}(3)$ размерности $2l+1$, и любое неприводимое n-мерное представление $\mathfrak{so}(3)$ изоморфно представлению ρ_l с $l = \frac{n-1}{2}$.

(?????) Для полуцелых l представления ρ_l не интегрируемы: они порождают двузначные представления SO(3), так называемые спинорные представления. Однако рассматриваемые как представления алгебры Ли $\mathfrak{su}(2) \simeq \mathfrak{so}(3), \rho_l$ соответствуют неприводимым унитарным представлениям группы Ли SU(2). Из теории представлений SU(2) следует, что при $l, l' \in \frac{1}{2}\mathbb{Z}_{\geqslant 0}$

$$V_l \otimes V_{l'} = \bigoplus_{j=|l-l'|}^{l+l'} V_j \qquad \text{(разложение Клебша-Гордона)}$$

Регулярное представление R группы SO(3) в $\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{x})$ не является неприводимым. Имеем

$$\mathscr{H} = L^2\left(S^2, d\boldsymbol{n}\right) \otimes L^2\left(\mathbb{R}_{>0}, r^2 dr\right),$$

$d\boldsymbol{n}$ - мера на S^2, индуцированная мерой Лебега на $\mathbb{R}^3$. Группа SO(3) действует вращениями на $L^2(S^2, d\boldsymbol{n})$, а на второй сомножитель она действует как тождественный оператор.

Таким образом, задача разложения регулярного представления R сводится к нахождению SO(3)-инвариантных подпространств гильбертова пространства $L^2\left(S^2, d\boldsymbol{n}\right)$. Итог:

$$L^2\left(S^2, d\boldsymbol{n}\right) = \bigoplus_{l=0}^{\infty} \mathscr{D}_l$$

$\mathscr{D}_l \simeq V_l$. (???????)

При этом изоморфизме ортонормированный базис Y_{lm} в $\mathscr{D}_l$, соответствующий базису e_{lm} в V_l, дается нормированными сферическими функциями

$$Y_{lm}(\vartheta, \varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} P_l^m(\cos\vartheta), \qquad m = -l, ..., l,$$

$$P_l^m(x) := (-1)^m \sqrt{\frac{(l+m)!}{(l-m)!}} \sqrt{\frac{2l+1}{2}} \frac{1}{2^l l!} \left(1-x^2\right)^{-\frac{m}{2}} \frac{d^{l-m}}{dx^{l-m}} \left(x^2-1\right)^l, \quad |x| < 1.$$

других операторах и величинах

О силе и определении величины силы (!??!??!?)

(абзац про то, как считать, с какой силой частица действует на стенки ямы???? пока остался вопрос. типа производную по энергии мб взять нужно и написать, что формализм, что только так и считаем?)

О времени и операторе времени

(1/3 страницы добавлю, смотрел статью про это, в теории подробнее напишу)

членах взаимодействия в гамильтониане (!?!?!??)

(show how to Construct quantum models!!!)

(тут член дипольного вз-я)

(тут член магнитного вз-я)

(??? какие еще есть???)

1.1.4 Density Matrix, Basics of Open Systems, SF

Density Matrix

(write what is it)

Basics of Open Systems, SF

$$\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}}, \quad Z = \mathrm{Tr}\left(e^{-\beta \hat{H}}\right) = \sum_n e^{-\beta E_n}$$

1.1.5 Relativistic quantum fields, QED: main laws

(see note on qft and field theory for now about it)

Об разложении $S-$матрицы в диаграммный ряд

Об уравнении Дирака

$$\mathcal{S}(x,y) = \langle 0|\ \mathrm{T}(\widehat{\psi}(x)\widehat{\bar{\psi}}(y))|0\rangle = \int \frac{\mathrm{d}^4 p}{(2\pi)^4} \mathrm{e}^{-\mathrm{i}p\cdot(x-y)} \frac{\mathrm{i}}{p^2 - m^2 + \mathrm{i}0}(\not{p} + m).$$

(Абзац О выводе уравнения Дирака из представлений группы Пуанкаре)

нерелятивистском пределе в сферическом потенциале и уравнению Паули

$$(\not{\mathcal{P}} - mc)\psi = 0, \qquad \mathcal{P}_k = \mathrm{i}\hbar\partial_k - \frac{e}{c}\mathcal{A}_k$$

$$\psi(t,\boldsymbol{r}) \equiv e^{-\frac{\mathrm{i}}{\hbar}mc^2 t}\begin{pmatrix}\varphi(t,\boldsymbol{r})\\ \chi(t,\boldsymbol{r})\end{pmatrix},$$

$$\begin{pmatrix} p_0 - \frac{e}{c}\phi - mc & (\boldsymbol{\sigma}\cdot\mathcal{P}) \\ -(\boldsymbol{\sigma}\cdot\mathcal{P}) & -p_0 + \frac{e}{c}\phi - mc\end{pmatrix}\begin{pmatrix}\varphi\\ \chi\end{pmatrix} = 0$$

$$p_0 := mc + \hat{\epsilon}/c, \qquad \hat{\epsilon} := \mathrm{i}\hbar\partial_t.$$

$$\chi = -\frac{1}{1 + \frac{\hat{\epsilon} - e\phi}{2mc^2}}\frac{(\boldsymbol{\sigma}\cdot\mathcal{P})}{2mc}\varphi,$$

$$\hat{\mathcal{W}} := \left|\frac{\hat{\epsilon} - e\Phi}{2mc^2}\right| \ll 1, \qquad \chi = -(1+\hat{\mathcal{W}})\frac{(\boldsymbol{\sigma}\cdot\mathcal{P})}{2mc}\varphi$$

$$\chi \ll \varphi \qquad \text{as} \qquad \mathcal{O}(v/c),$$

Получаем действие Дирака через ψ: (??? перерешаю!)

$$c\bar{\psi}(\not{\mathcal{P}} - mc)\psi = \varphi^\dagger\{(\hat{\epsilon} - e\phi)\varphi + c(\boldsymbol{\sigma}\cdot\mathcal{P})\chi\} = \varphi^\dagger\left\{\hat{\epsilon} - e\phi - \frac{1}{2m}(\boldsymbol{\sigma}\cdot\mathcal{P})(1+\hat{\mathcal{W}})(\boldsymbol{\sigma}\cdot\mathcal{P})\right\}\varphi$$

$S_{\mathrm{NR}} = \int dt \int d^3\boldsymbol{r}\varphi^\dagger\left\{\hat{\epsilon} - e\phi - \frac{1}{2m}(\boldsymbol{\sigma}\cdot\mathcal{P})^2\right\}\varphi$, $(\boldsymbol{\sigma}\cdot\mathcal{P})^2 = \mathcal{P}^2 + \mathrm{i}\boldsymbol{\sigma}(\mathcal{P}\times\mathcal{P})$, $\mathcal{P}_\beta = -\mathrm{i}\hbar\partial_\beta - \frac{e}{c}\mathcal{A}_\beta \Rightarrow$ $(\mathcal{P}\times\mathcal{P}) = \mathrm{i}\frac{\hbar e}{c}\mathcal{H}$,

$$S_{\mathrm{Pauli}} = \int dt \int d^3\boldsymbol{r}\varphi^\dagger\left\{\hat{\epsilon} - e\phi - \frac{\mathcal{P}^2}{2m} + \frac{e\hbar}{2mc}(\boldsymbol{\sigma}\cdot\boldsymbol{\mathcal{H}})\right\}\varphi$$

$$i\hbar\frac{\partial}{\partial t}\varphi = \hat{H}_{\mathrm{Pauli}}\varphi, \qquad \hat{H}_{\mathrm{Pauli}} := \frac{\mathcal{P}^2}{2m} + e\phi - g\frac{e\hbar}{2mc}(s\cdot\mathcal{H}),$$

$s := \frac{1}{2}\sigma$, $g := 2$.

Релятивистские поправки для статического потенциала (???)

(???)

В случае $\mathcal{A} = 0$

$$ej^0 \approx e\varphi^\dagger\left\{1 + \frac{\boldsymbol{p}^2}{4m^2c^2}\right\}\varphi$$

Об уравнении Клейна-Гордона

(пока в теорполе, потом это же тут и будет)

Об уравнениях Максвелла и формул о фотонах для задач квантовой механики

(или тут, или в разделе о связке с КТП это напишу, пока тут, так проще.)

Другое о релятивистской квантовой механике

(тут обзор основных моделей и применений уравнений. подробно - в одной из следующих частях)

Уравнение Дирака для позитрона

(пока еще не разобрался полностью)
(абзац, почему не достаточно просто заменить e на -e? тонкости такие есть...)

Idea and main formulas of QED

(см. пока запись по КТП, потом сюда тоже добавлю.)

Расходимость рядов в квантовой электродинамике по МК

1.1.6 Spin, spinors, γ-matrices

Main physical properties of a spin

Спин можно определять аксиоматически:
A10 (Частицы со спином). Гильбертово пространство состояний квантовой частицы спина $s \in \left\{0, \frac{1}{2}, 1, \frac{3}{2}, ...\right\}$ - это $\mathscr{H}_S = L^2\left(\mathbb{R}^3\right) \otimes V_s$, $V_s - 2s + 1$-мерное комплексное векторное пространство неприводимого представления R_s группы Ли SU(2) спина s. Операторы спина $S = (S_1, S_2, S_3)$ даются формулой

$$S_j = i\hbar\rho_s\left(A_j\right), \quad j = 1, 2, 3,$$

A_1, A_2, A_3 - стандартные образующие алгебры Ли $\mathfrak{su}(2)$, а $\rho_s = dR_s$ - соответствующее представление $\mathfrak{su}(2)$ в V_s. Частицы с целым спином называются бозонами, а с полуцелым спином - фермионами.

Connection of a Spin and Orbital Angular Momentum

$$\boldsymbol{\mu} = \frac{q}{2mc}\mathbf{L} \qquad \text{gyromagnetic}$$

$$\boldsymbol{\mu} = g\frac{q}{2mc}\mathbf{S}$$

$$\boldsymbol{\mu} = g\mu_N\mathbf{S}, \quad \mu_N = \frac{q}{2m_pc}$$

$$g_p \approx 5.56, \quad g_n \approx -3.83$$

Построение нерелятивистских спиноров, алгебра $su(2)$, спиновые матрицы

Основные методы и формулы о спинах

Спина строится как представление алгебры $su(2)$. А именно: пусть $A_1 = -\frac{i}{2}\sigma_1$, $A_2 = -\frac{i}{2}\sigma_2$, $A_3 = -\frac{i}{2}\sigma_3$ - стандартный базис алгебры Ли su(2) - алгебры 2×2 косоэрмитовых матриц с нулевым следом, у них $[A_1, A_2] = A_3$, $[A_2, A_3] = A_1$, $[A_3, A_1] = A_2$, и пусть $\rho_{\frac{1}{2}}$ - двумерное (фундаментальное) представление $\mathfrak{su}(2)$ в $V_{\frac{1}{2}} \simeq \mathbb{C}^2$. Операторы спина даются формулами

$$S_j = i\hbar\rho_{\frac{1}{2}}(A_j), \quad j = 1, 2, 3$$

и $\rho_{\frac{1}{2}}$ называется представлением спина $\frac{1}{2}$.

В общем, представление ρ_s в $2s+1$-мерном комплексном векторном пространстве V_s называется представлением спина $s \in \frac{1}{2}\mathbb{Z}_{\geqslant 0}$. Действие операторов $T_j = i\rho_s(A_j)$ на V_s описывается формулами

$$\begin{aligned}(T_1 - iT_2)\, e_{sm} &= -\sqrt{(s+m)(s-m+1)}\, e_{sm-1}\\ (T_1 + iT_2)\, e_{sm} &= -\sqrt{(s-m)(s+m+1)}\, e_{sm+1}\\ T_3 e_{sm} &= m e_{sm}.\end{aligned}$$

(абзац про то, что орбитальный момент и спин это разные вещи (???) важный вопрос)

Целость и полуцелость спина (квантование спина)

Потому что если мы посчитаем квадрат $N^2 := s_\mp s_\pm$, то он окажется равным $\lambda_s - m_s(m_s \pm 1)$, при этом собственных векторов конечное число, отсюда и квантование.

(??а почему N^2 должен быть положительный???)

$$\begin{aligned}\boldsymbol{s}^2 = s_x^2 + s_y^2 + s_z^2 = s_+ s_- + \mathrm{i}\,[s_x, s_y] + s_z^2 = s_+ s_- - s_z + s_z^2 \equiv\\ \equiv s_- s_+ - \mathrm{i}\,[s_x, s_y] + s_z^2 = s_- s_+ + s_z + s_z^2.\end{aligned}$$

$$\begin{aligned}\langle \lambda_s, m_s | s_\mp s_\pm | \lambda_s, m_s\rangle = (s_\pm |\lambda_s, m_s\rangle)^\dagger\, s_\pm |\lambda_s, m_s\rangle = N_\pm^2(\lambda_s, m_s) \equiv\\ \equiv \left\langle \lambda_s, m_s \middle| \left(s^2 - s_z^2 \mp s_z\right)\right| \lambda_s, m_s\right\rangle = \lambda_s - m_s(m_s \pm 1).\end{aligned}$$

Поэтому

$$\begin{gathered}m_s(m_s \pm 1) \leqslant \lambda_s,\\ m_s^{\max}(m_s^{\max}+1) - m_s^{\min}\left(m_s^{\min} - 1\right) = 0,\\ m_s^{\max}(m_s^{\max}+1) - (m_s^{\max} - n)(m_s^{\max} - n - 1) = 0,\\ m_s^{\max} = \frac{n}{2}, \qquad m_s^{\min} = -\frac{n}{2}.\\ s := m_s^{\max} = \frac{n}{2},\end{gathered}$$

О спинорной метрике (???)

(чуть потренирую - и напишу, не так это нужно особо)

$$\hat\epsilon \stackrel{\text{def}}{=} \begin{pmatrix} 0 & 1\\ -1 & 0\end{pmatrix} = \mathrm{i}\sigma_2, \quad \hat\epsilon^2 = -\mathbb{1}, \quad \hat\epsilon^{-1} = \hat\epsilon^{\mathrm{T}} = -\hat\epsilon$$

$$\psi_c \stackrel{\text{def}}{=} -\hat\epsilon\psi^* = -\mathrm{i}\sigma_2\psi^*,$$

(? почему именно она?)

$$\hat{\epsilon}\circ\exp\{A\}\circ\hat{\epsilon}^{-1}=\hat{\epsilon}\circ\left(\sum_{n=0}^{\infty}\frac{1}{n!}A^n\right)\circ\hat{\epsilon}^{-1}=\sum_{n=0}^{\infty}\frac{1}{n!}\left\{\hat{\epsilon}\circ A\circ\hat{\epsilon}^{-1}\right\}^n=\exp\left\{\hat{\epsilon}\circ A\circ\hat{\epsilon}^{-1}\right\}.$$

$$\hat{R}_S=\exp\left(-\frac{\mathrm{i}}{2}\phi(\boldsymbol{\sigma}\cdot\mathcal{O})\right)$$
$$\hat{R}^*_S=\exp\left(\frac{\mathrm{i}}{2}\phi\left(\boldsymbol{\sigma}^*\cdot\mathcal{O}\right)\right).$$

(??? место додумать!)

(????) Сопряженный спинор при поворотах преобразуется также, как и обычный спинор. Поэтому скаляром будет величина

$$-\chi^\dagger\cdot\psi_c=-\bar{\chi}_{\dot{\alpha}}\bar{\psi}^{\dot{\alpha}}$$

$$\bar{\chi}_{\dot{\alpha}}=\left(\chi^\dagger\right)_{\dot{\alpha}}$$
$$\chi^\dagger=\{\chi^*\}^{\mathrm{T}}=\{\hat{\epsilon}\,(-\hat{\epsilon}\chi^*)\}^{\mathrm{T}}=\{\hat{\epsilon}\bar{\chi}\}^{\mathrm{T}}=-\bar{\chi}^{\mathrm{T}}\hat{\epsilon}$$

Поэтому

$$-\bar{\chi}\cdot\bar{\psi}=\bar{\chi}^{\mathrm{T}}\hat{\epsilon}\bar{\psi}=\bar{\chi}^{\dot{\alpha}}\epsilon_{\dot{\alpha}\dot{\beta}}\bar{\psi}^{\dot{\beta}},\quad \epsilon_{12}=1,$$

т.е. метрика $\epsilon_{\dot{\alpha}\dot{\beta}}$ в спинорных индексах с точкой совпадает с метрикой $\epsilon_{\alpha\beta}$ в спинорных индексах без точек.

спинорах

(коротко, потому что подробнее в теории поля.)

О спиральности (?????)

(!?!!!! еще раз про спин фотона подумаю, так и не понял, если мы говорим, что спин это генератор группы вращений, то что с фотоном то делать???? как представить его вращения???? мы же даже в его систему не можем перейти ведь???? пока хз)

$$\gamma^0=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix},\qquad \gamma^1=\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&-1&0&0\\-1&0&0&0\end{pmatrix},\qquad \gamma^2=\begin{pmatrix}0&0&0&-i\\0&0&i&0\\0&i&0&0\\-i&0&0&0\end{pmatrix},$$
$$\gamma^3=\begin{pmatrix}0&0&1&0\\0&0&0&-1\\-1&0&0&0\\0&1&0&0\end{pmatrix}.\qquad I_4=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix},\quad \gamma^5\equiv i\gamma^0\gamma^1\gamma^2\gamma^3=\begin{pmatrix}0&0&1&0\\0&0&0&1\\1&0&0&0\\0&1&0&0\end{pmatrix}$$

$(\gamma^0)^\dagger=\gamma^0$
$\gamma^0\gamma^\mu\gamma^0=(\gamma^\mu)^\dagger,$

$$\gamma_\lambda\gamma^\lambda = 4,$$
$$\gamma_\lambda\gamma^\alpha\gamma^\lambda = -2\gamma^\alpha$$
$$\gamma_\lambda\gamma^\alpha\gamma^\beta\gamma^\lambda = 4g^{\alpha\beta},$$
$$\gamma_\lambda\gamma^\alpha\gamma^\beta\gamma^\gamma\gamma^\lambda = -2\gamma^\gamma\gamma^\beta\gamma^\alpha$$
$$\gamma_i\gamma^\alpha\gamma^\beta\gamma^\gamma\gamma^\delta\gamma^\lambda = 2\left(\gamma^\delta\gamma^\alpha\gamma^\beta\gamma^\gamma + \gamma^\gamma\gamma^\beta\gamma^\alpha\gamma^\delta\right)$$

For 4-vectors A, B: $\gamma_\lambda \not{A}\gamma^\lambda = -2\not{A}$ $\quad \not{A} := \gamma^\alpha A_\alpha$

$$\gamma_\lambda \not{A}\not{B}\gamma^\lambda = 4\not{A}\not{B},$$
$$\gamma_\lambda \not{A}\not{B}\not{C}\gamma^\lambda = -2\not{C}\not{B}\not{A}$$
$$\gamma_\lambda \not{A}\not{B}\not{C}\not{D}\gamma^\lambda = 2(\not{D}\not{A}\not{B}\not{C} + \not{C}\not{B}\not{A}\not{D})$$

$$\mathrm{Tr}(\not{A}\not{B}) = 4(AB)$$
$$\mathrm{Tr}(\not{A}\not{B}\not{C}\not{D}) = 4\{(AB)(CD) - (AC)(BD) + (AD)(BC)\},$$
$$\mathrm{Tr}\left(\not{A}_1\not{A}_2...\not{A}_{2n}\right) = (A_1A_2)\,\mathrm{Tr}\left(\not{A}_3...\not{A}_{2n}\right) - (A_1A_3)\,\mathrm{Tr}\left(A_2A_4...A_{2n}\right) + ... + (A_1A_{2n})\,\mathrm{Tr}\left(\not{A}_2\not{A}_3...\not{A}_{2n-1}\right).$$

$$\not{A}\not{B} = AB - \mathrm{i}\sigma^{\alpha\beta}A_\alpha B_\beta = 2AB - \not{B}\not{A},$$
$$\not{A}\not{A} = A^2; \qquad \text{if } AB = 0. \qquad \not{A}\not{B} = -\not{B}\not{A},$$

(i) For any two $n \times n$ matrices U, V we have: $\mathrm{Tr}(UV) = \mathrm{Tr}(VU)$
(ii) If $\left(\gamma^\alpha\gamma^\beta\cdots\gamma^\mu\gamma^\nu\right)$ contains an odd number of γ-matrices: $\mathrm{Tr}\left(\gamma^\alpha\gamma^\beta\cdots\gamma^\mu\gamma^\nu\right) = 0$
(iii) For a product of an even number of γ-matrices:

$$\mathrm{Tr}\left(\gamma^\alpha\gamma^\beta\right) = 4g^{\alpha\beta}, \quad \mathrm{Tr}\,\sigma^{\alpha\beta} = 0$$
$$\mathrm{Tr}\left(\gamma^\alpha\gamma^\beta\gamma^\gamma\gamma^\delta\right) = 4\left(g^{\alpha\beta}g^{\gamma\delta} - g^{\alpha\gamma}g^{\beta\delta} + g^{\alpha\delta}g^{\beta\gamma}\right),$$

(iv) For any product of γ-matrices

$$\mathrm{Tr}\left(\gamma^\alpha\gamma^\beta...\gamma^\mu\gamma^\nu\right) = \mathrm{Tr}\left(\gamma^\nu\gamma^\mu...\gamma^\beta\gamma^\alpha\right)$$

$$\mathrm{Tr}\left(\not{A}_1\not{A}_2...\not{A}_{2n}\right) = \mathrm{Tr}\left(\not{A}_{2n}...\not{A}_2\not{A}_1\right)$$

$$\mathrm{Tr}\,\gamma^5 = \mathrm{Tr}\left(\gamma^5\gamma^\alpha\right) = \mathrm{Tr}\left(\gamma^5\gamma^\alpha\gamma^\beta\right) = \mathrm{Tr}\left(\gamma^5\gamma^\alpha\gamma^\beta\gamma^\gamma\right) = 0$$
$$\mathrm{Tr}\left(\gamma^5\gamma^\alpha\gamma^\beta\gamma^\gamma\gamma^\delta\right) = -4\mathrm{i}\varepsilon^{\alpha\beta\gamma\delta}$$

$\left(\gamma^5\right)^2 = 1,$

$$\mathrm{Tr}\left(\gamma^\alpha...\gamma^\nu\right) = \mathrm{Tr}\left[\left(\gamma^5\right)^2\gamma^\alpha...\gamma^\nu\right] = \mathrm{Tr}\left(\gamma^5\gamma^\alpha...\gamma^\nu\gamma^5\right)$$

Algebra of $\mathfrak{su}(2)$ and spins

$\mathscr{H}_S = \mathscr{H} \otimes \mathbb{C}^2,$
$\Psi = \begin{pmatrix} \psi_1(\boldsymbol{x}) \\ \psi_2(\boldsymbol{x}) \end{pmatrix} \in \mathscr{H}_S, \qquad \|\Psi\|^2 = \int\limits_{\mathbb{R}^3} |\psi_1(\boldsymbol{x})|^2\, d^3\boldsymbol{x} + \int\limits_{\mathbb{R}^3} |\psi_2(\boldsymbol{x})|^2\, d^3\boldsymbol{x} < \infty.$

Каждой наблюдаемой A в $\mathscr{H}$ соответствует наблюдаемая $A \otimes I_2$ в $\mathscr{H}_S$, задаваемая 2×2 блочно-диагональной матрицей $\begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix}$. Наблюдаемые вида $I \otimes S$, I - тождественный

оператор в $\mathscr{H}$, а S - самосопряженный оператор в $\mathbb{C}^2$, описывают внутренние степени свободы и коммутируют со всеми наблюдаемыми $A \otimes I_2$. Полный набор наблюдаемых в $\mathscr{H}_S$ состоит из операторов $Q_1 \otimes I_2, Q_2 \otimes I_2, Q_3 \otimes I_2$ и $I \otimes S_1, I \otimes S_2, I \otimes S_3$, Q_j - операторы координат, а S_j - операторы спина, самосопряженные операторы в $\mathbb{C}^2$ с нулевым следом, удовлетворяющие тем же коммутационным соотношениям, что и квантовые операторы углового момента,

$$[S_1, S_2] = i\hbar S_3, \quad [S_2, S_3] = i\hbar S_1, \quad [S_3, S_1] = i\hbar S_2.$$

В стандартном базисе $e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ пространства $\mathbb{C}^2$, $S_j = \frac{\hbar}{2}\sigma_j, j = 1, 2, 3$, σ_j - это матрицы Паули:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Тут σ_z - это с.з. на диагонали, а другие восстанавливаются из σ_+, σ_-, у которых только одна 1 на крос-диагонали.

Часто представляем $\Psi \in \mathscr{H}_S$ как функцию $\psi(\boldsymbol{x}, \sigma)$, $\boldsymbol{x} \in \mathbb{R}^3$, а $\sigma \in \{\frac{1}{2}, -\frac{1}{2}\}$, положив $\psi\left(\boldsymbol{x}, \frac{1}{2}\right) = \psi_1(\boldsymbol{x})$ и $\psi\left(\boldsymbol{x}, -\frac{1}{2}\right) = \psi_2(\boldsymbol{x})$. Каждая функция $\psi(\boldsymbol{x}, \sigma)$ является конечной линейной комбинацией функций $\psi(\boldsymbol{x})\chi(\sigma)$ - разложимых на множители элементов тензорного произведения $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$. Мы отождествляем $\mathbb{C}^2$ с комплексным векторным пространством функций $\chi : \left\{-\frac{1}{2}, \frac{1}{2}\right\} \to \mathbb{C}$, сопоставляя стандартному базису e_1, e_2 функции χ_1, χ_2, определенные формулами $\chi_1\left(\frac{1}{2}\right) = 1, \chi_1\left(-\frac{1}{2}\right) = 0$ и $\chi_2\left(\frac{1}{2}\right) = 0, \chi_2\left(-\frac{1}{2}\right) = 1$.

su(2) main properties

(see note about algebra for now!)

$$J_\pm = J_1 \pm iJ_2, \quad [J_3, J_\pm] = \pm\hbar J_\pm, \quad [J_+, J_-] = 2\hbar J_3, \quad \left[J^2, J_\pm\right] = 0$$

$$J^2 = \frac{1}{2}(J_+J_- + J_-J_+) + J_3^2, \quad J_-J_+ = J^2 - J_3(J_3 + \hbar), \quad J_+J_- = J^2 - J_3(J_3 - \hbar)$$

$$J_+|jm\rangle = \hbar\sqrt{(j-m)(j+m+1)}|j, m+1\rangle, \quad J_-|jm\rangle = \hbar\sqrt{(j+m)(j-m+1)}|j, m-1\rangle.$$

$$|jm\rangle = \sqrt{\frac{(j+m)!}{(2j)!(j-m)!}}\left(\frac{J_-}{\hbar}\right)^{j-m}|jj\rangle$$

$$\langle j'm'|\, J_3|jm\rangle = \hbar\delta_{j'j}\delta_{m'm}m$$

О матрицах Паули

$$\sigma_1 = \sigma_{\mathrm{x}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \sigma_{\mathrm{y}} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_3 = \sigma_{\mathrm{z}} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

They can be restored from s_z and s_+, s_-.

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \equiv \frac{\hbar}{2}[(|\uparrow\rangle\langle\downarrow|) + (|\downarrow\rangle\langle\uparrow|)]; \qquad \hat{S}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \equiv \frac{i\hbar}{2}[-(|\uparrow\rangle\langle\downarrow|) + (|\downarrow\rangle\langle\uparrow|)]$$

$$\begin{aligned}\sigma_x \cos\varphi + \sigma_y \sin\varphi =& e^{-i\varphi\sigma_z/2}\sigma_x e^{i\varphi\sigma_z/2},\\ \sigma_x \sin\varphi - \sigma_y \cos\varphi =& -e^{-i\varphi\sigma_z/2}\sigma_y e^{i\varphi\sigma_z/2}.\end{aligned}$$

О $s = 1$ матрицах

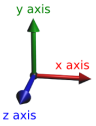
$$s_x = \mathrm{i}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \qquad s_y = \mathrm{i}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \qquad s_z = \mathrm{i}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

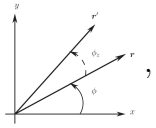
$$[s_i, s_j] = \mathrm{i}\varepsilon_{ijk}s_k.$$

$$s^2\,|\lambda_s, m_s\rangle = \lambda_s\,|\lambda_s, m_s\rangle\,, \quad s_z\,|\lambda_s, m_s\rangle = m_s\,|\lambda_s, m_s\rangle\,.$$

$$s_\pm = s_x \pm \mathrm{i}\ s_y$$

$$\left[s^2, s_\pm\right] = 0$$

Restore the position of two ± 1 in $\hat{s}_{s_{x,y,z}}$ by: 

$\Rightarrow$  ,

$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\phi_z & -\sin\phi_z \\ \sin\phi_z & \cos\phi_z \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix}$, $\quad \hat{G}(\boldsymbol{a}) \approx \mathbb{1} - \mathrm{i}\Gamma_\alpha a^\alpha, \quad \Gamma_\alpha := \mathrm{i}\lim_{\boldsymbol{a}\to 0}\frac{\partial}{\partial a^\alpha}\hat{T}(\boldsymbol{a})$.

(?? додумаю, для больших спинов такой метод не работает, а почему? вообще, укажу про большие спины тут!)

Об индексах и их позиции

(см. пока теорпол, потом сюда тоже допишу)

(???? абзац про точечный и неточечный индексы, что это и зачем???)

Wigner D-matrix basics (?)

$$D^j_{m'm}(U) = \langle jm'|\,U|jm\rangle$$

$$D^j_{mm'}(\alpha,\beta,\gamma) = \langle jm|e^{-i\alpha J_z/\hbar}e^{-i\beta J_y/\hbar}e^{-i\gamma J_z/\hbar}\,|jm'\rangle$$

$$D^j_{mm'}(\alpha,\beta,\gamma) = e^{-i\alpha m - i\gamma m'}d^j_{mm'}(\beta), \quad d^j_{mm'}(\beta) = \langle jm|e^{-i\beta J_y/\hbar}|jm\rangle$$

$$D^j_{mm'}\left(U^{-1}\right) = D^{j*}_{m'm}(U)$$

(see wiki for now)

On higher spin representations of $su(2)$

(see algebra for now.)

Спиновые матрицы плотности (from Vergeles)

Спиновые матрицы плотности необходимы при вычислении сечений и вероятностей распадов, т.к. в процессе таких вычислений приходится делать замены выражений, билинейных относительно спиновых волновых функций начальных и конечных частиц, согласно правилу

$$e_{\mathbf{k}\mu}e^*_{\mathbf{k}\nu} \longrightarrow \rho_{\mu\nu}(k), \quad u_{\pm ka}\bar{u}_{\pm kb} \longrightarrow \rho^{(\pm)}_{ab}(k) \tag{Б1}$$

где $\rho_{\mu\nu}(k)$ - спиновая матрица плотности фотона, $\rho^{(+)}_{ab}(k)\left(\rho^{(-)}_{ab}(k)\right)$ - спиновая матрица плотности электрона (позитрона), причём импульс всех этих частиц равен $\mathbf{k}$.

Фотонные спиновые матрицы плотности.

$$\rho^{\text{unpol}}_{ij} = \frac{1}{2}\left(\delta_{ij} - \frac{k_i k_j}{\mathbf{k}^2}\right), \quad \rho_{0i} = \rho_{i0} = \rho_{00} = 0 \tag{Б2}$$

$$\rho^{\mu}_{\mu} = -1 \tag{Б3}$$

$$\rho_{\mu\nu}(k) \longrightarrow \rho_{\mu\nu}(k) + (\chi_\mu k_\nu + \chi_\nu k_\mu) \tag{Б4}$$

$$\chi^\mu = \left(-\frac{1}{4\omega}, \frac{\mathbf{k}}{4\omega^2}\right) \qquad \Rightarrow \qquad \rho_{\mu\nu} = -\eta_{\mu\nu}/2 \tag{Б5}$$

В общем случае матрица плотности представляется в виде

$$\rho_{\mu\nu} = \rho^*_{\nu\mu} = \sum_{\alpha,\beta=1}^{2} \rho^{\alpha\beta} e_{\alpha\mu} e^*_{\beta\nu} \tag{Б6}$$

$$\rho^{\alpha\beta} = \rho^{\beta\alpha *} \tag{Б7}$$

$$\rho^{\alpha\beta}_{\text{unpol}} = (1/2)\delta^{\alpha\beta} \tag{Б8}$$

$$\det \rho^{\alpha\beta}_{\text{unpol}} = 1/4 \tag{Б9}$$

$$\rho^{\alpha\beta}_{\text{fully pol}} = v^\alpha v^{\beta *} \tag{В10}$$

$$\det \rho^{\alpha\beta}_{\text{fully pol}} = 0 \tag{Б11}$$

В общем случае:

$$\sum_{\alpha=1}^{2} \rho^{\alpha\alpha} = 1 \tag{Б12}$$

$$0 \leq \det \rho^{\alpha\beta} \leq 1/4 \tag{Б13}$$

$$\rho = \frac{1}{2}(1 + \boldsymbol{\xi}\boldsymbol{\sigma}), \quad \boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3) \tag{Б14}$$

$$\det \rho = \frac{1}{4}\left(1 - \xi_1^2 - \xi_2^2 - \xi_3^2\right) \tag{Б15}$$

$$0 \le \xi_1^2 + \xi_2^2 + \xi_3^2 \equiv \boldsymbol{\xi}^2 \le 1 \tag{Б16}$$

Поэтому в неполяризованном случае $\xi^2 = 0$, а в полностью поляризованном $\xi^2 = 1$.

Спинорные матрицы плотности.

$$\operatorname{tr} \rho^{(\pm)}(k) = \pm 2m \tag{Б19}$$

$$(\not{k} \mp m)\rho^{(\pm)}(k) = \rho^{(\pm)}(k)(\not{k} \mp m) = 0 \tag{Б20}$$

$$\langle \mathbf{s} \rangle = \frac{1}{2\omega_k} \operatorname{tr}\left(\rho^{(\pm)}\gamma^0 \boldsymbol{\Sigma}\right) = \frac{1}{4\omega_k} \operatorname{tr}\left(\rho^{(\pm)}\gamma^5\gamma\right) \tag{Б21}$$

Матрица плотности для неполяризованного состояния получается при $\frac{1}{2}\sum\limits_{s=1,2} u_{\pm ks}\bar{u}_{\pm ks} = \not{k} \pm m$

$$\rho^{(\pm)}(k) = (1/2)(\not{k} \pm m) \tag{Б22}$$

В общем случае

$$\rho^{(\pm)}(k) = (1/2)(\not{k} \pm m)\left(1 - \gamma^5 \not{a}\right) \tag{Б23}$$

$a^\mu: \quad k_\mu a^\mu = 0 \quad \longleftrightarrow \quad \not{a}\not{k} + \not{k}\not{a} = 0$

$$\pm a^\mu = \frac{1}{2m} \operatorname{tr}\left(\rho^{(\pm)}\gamma^5\gamma^\mu\right) \tag{b25}$$

В системе покоя частицы

$$a^\mu = (0, \pm 2\langle \mathbf{s} \rangle) \tag{Б26}$$

$0 \le \langle \mathbf{s} \rangle^2 \le 1/4 \quad \Rightarrow -1 \le a^2 \le 0$

Также в сечение рассеяния следует внести дополнительный множитель 2^r, где r - суммарное число электронов, позитронов и фотонов в конечном состоянии. Этот множитель означает учёт обоих состояний спина каждой конечной частицы. (??)

других темах про спин

(просто укажу тут их, их прямо очень много, но я не буду их касаться, так что эти разделы дальше, на которые тут будет отсылка, вряд ли создам скоро.)

связи спина со статистикой

bosons: $\left[\mathfrak{a}^\dagger_\lambda(\boldsymbol{k}), \mathfrak{a}^\dagger_{\lambda'}(\boldsymbol{k}')\right] = 0 \qquad [\mathfrak{a}_\lambda(\boldsymbol{k}), \mathfrak{a}_{\lambda'}(\boldsymbol{k}')] = 0$

femions: $\left\{\mathfrak{a}^\dagger_\lambda(\boldsymbol{k}), \mathfrak{a}^\dagger_{\lambda'}(\boldsymbol{k}')\right\} = 0 \qquad \{\mathfrak{a}_\lambda(\boldsymbol{k}), \mathfrak{a}_{\lambda'}(\boldsymbol{k}')\} = 0$

(тут про вывод, почему так? (!?!???))
(тут про то, что видите ли, в КТП могут быть госты, у которых это не так.)

другом про спиноры

1.1.7 Information, entanglement, entropy

(свяжу потом с записью по кв теор инф!)

(see Tong!!!! просто пока это не нужно было и сейчас не нужно, пару дней подумаю - и готов буду написать)

Quantum Maps

$$\rho = \mathrm{Tr}_{\mathcal{H}_E} |\Psi\rangle\langle\Psi|$$

We would like to understand how this density matrix evolves. The state $|\Psi\rangle$ evolves by a unitary operator $U(t)$ acting on the full Hilbert space $\mathcal{H}$. The story that we are about to tell only works if, at time $t = 0$, the two systems lie in a separable state,

$$|\Psi_0\rangle = |\psi\rangle \otimes |\chi\rangle$$

This means that the original density matrix $\rho_0 = |\psi\rangle\langle\psi|$ describes a pure state on $\mathcal{H}_S$. We now look at how this density matrix evolves. We have

$$\rho(t) = \mathrm{Tr}_{\mathcal{H}_E} U(t) |\Psi_0\rangle \langle\Psi_0| U^\dagger(t) = \sum_m \langle m|U(t) |\Psi_0\rangle \langle\Psi_0| U^\dagger(t)|m\rangle$$

with $|m\rangle$ a complete basis for $\mathcal{H}_E$. This encourages us to define a set of operators on $\mathcal{H}_S$, given by

$$M_m(t) = \langle m|U(t)|\chi\rangle = \mathrm{Tr}_{\mathcal{H}_E}(U(t)|\chi\rangle\langle m|)$$

The unitarity of $U(t)$ translates into a completeness condition on the operators $M_m(t)$,

$$\sum_m M_m^\dagger(t) M_m(t) = \sum_m \langle\chi|U^\dagger(t)|m\rangle\langle m|U(t)|\chi\rangle = 1$$

We see that the original density matrix on $\mathcal{H}_S$ evolves as

$$\rho(t) = \sum_m M_m(t)\rho_0 M_m^\dagger(t)$$

Kraus Representation Theorem

$$\rho \mapsto \mathcal{L}[\rho]$$

Such a map is sometimes called a superoperator (because it maps operators to operators, rather than states to states). We will require some special properties of our map, most of which are inherited from the properties of the density matrices listed in Section 5.3

- Linearity: $\mathcal{L}[a\rho_1 + b\rho_2] = a\mathcal{L}[\rho_1] + b\mathcal{L}[\rho_2]$.
- Hermiticity Preserving: $\rho = \rho^\dagger \Rightarrow \mathcal{L}[\rho] = \mathcal{L}[\rho]^\dagger$.
- Trace Preserving: $\mathrm{Tr}\,\mathcal{L}[\rho] = \mathrm{Tr}\,\rho$.
- Complete Positivity. This one requires some explanation. It is natural to insist that the map is positive, so that $\mathcal{L}[\rho] \geq 0$ whenever $\rho \geq 0$. However, this is not sufficient. Instead, we require the stronger statement that the map $\mathcal{L} \otimes \mathbf{1}_E$ is positive on any extension of the Hilbert space $\mathcal{H}_S$ to $\mathcal{H}_S \otimes \mathcal{H}_E$. This is the statement of complete positivity. It ensures that the map $\mathcal{L} \otimes \mathbf{1}_E$ will take a valid density matrix on the composite system to another density matrix.

A superoperator obeying these conditions is called a trace preserving, completely positive (TPCP) map, with the first two conditions taken for granted. In the quantum information community, this map is referred to as a quantum channel.

The Kraus representation theorem (which we do not prove here) states that any quantum map, obeying the four conditions above, can be written as

$$\mathcal{L}[\rho] = \sum_m M_m \rho M_m^\dagger \quad \text{with} \quad \sum_m M_m^\dagger M_m = 1$$

In this framework, the M_m are called Kraus operators. They are not unique. The number of Kraus operators in the quantum map does not exceed $\dim(\mathcal{H}_S)^2$.

The CHSH Game

Dense Coding

Quantum Teleportation

Quantum Key Distribution

Об энтропии в квантовой механике

(!!!????)

The Increase of Entropy in quantum systems

$$S(\rho) = -\operatorname{Tr}\rho\log\rho$$

$$\frac{dS}{dt} = -\operatorname{Tr}\left(\frac{\partial\rho}{\partial t}(1+\log\rho)\right) = -\operatorname{Tr}\left(\frac{\partial\rho}{\partial t}\log\rho\right)$$

$$\hbar\frac{dS}{dt} = -\sum_m \operatorname{Tr}\left[(L_m\rho L_m - L_m L_m\rho)\log\rho\right]$$

$$\rho = \sum_i p_i \left|\phi_i\right\rangle\left\langle\phi_i\right|$$

$$\begin{aligned}\hbar\frac{dS}{dt} &= -\sum_m\sum_i \left\langle\phi_i\right|(L_m\rho L_m - L_m L_m\rho)\left|\phi_i\right\rangle\log p_i \\ &= -\sum_m\sum_{i,j}\left\langle\phi_i\right|L_m\left|\phi_j\right\rangle\left\langle\phi_j\right|L_m\left|\phi_i\right\rangle(p_j-p_i)\log p_i \\ &= -\frac{1}{2}\sum_m\sum_{i,j}\left|\langle\phi_i|L_m|\phi_j\rangle\right|^2(p_j-p_i)(\log p_i - \log p_j)\end{aligned}$$

$$\hbar\frac{dS}{dt} \geq 0$$

(??? и что с этим делать? статфиз говорил, что нет, такого не может быть???)

1.1.8 Path integral: basics

(только самое важное, пока в КТП об этом. страницы мб 5 будет.)

Main formulas to work with a path integral

Main ideas of path integral

$$K\left(x,t;x_0,t_0\right)=\langle x|U\left(t,t_0\right)|x_0\rangle$$

$$\psi(x,t)=\int dx_0 K\left(x,t;x_0,t_0\right)\psi\left(x_0,t_0\right)$$

$$U(\epsilon)=1-\frac{i\epsilon}{\hbar}(T+V)+O\left(\epsilon^2\right)=e^{-i\epsilon T/\hbar}e^{-i\epsilon V/\hbar}+O\left(\epsilon^2\right)$$

$$U(t)=\left(e^{-i\epsilon T/\hbar}e^{-i\epsilon V/\hbar}\right)^N+O(1/N)\qquad t=N\varepsilon$$

$$K\left(x,x_0,t\right)=\lim_{N\to\infty}\int dx_1...dx_{N-1}\prod_{j=0}^{N-1}\left\langle x_{j+1}\right|e^{-i\epsilon T/\hbar}e^{-i\epsilon V/\hbar}\left|x_j\right\rangle,\quad x=x_N$$

$$\int dp\left\langle x_{j+1}\right|e^{-i\epsilon\hat{p}^2/2m\hbar}|p\rangle\langle p|e^{-i\epsilon V(\hat{x})/\hbar}\left|x_j\right\rangle=\sqrt{\frac{m}{2\pi i\epsilon\hbar}}\exp\left[\frac{i}{\hbar}\left(m\frac{\left(x_{j+1}-x_j\right)^2}{2\epsilon}-\epsilon V\left(x_j\right)\right)\right]$$

$$K\left(x,x_0,t\right)=\lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2}\int dx_1...dx_{N-1}\exp\left[\frac{i\epsilon}{\hbar}\sum_{j=0}^{N-1}\left(m\frac{\left(x_{j+1}-x_j\right)^2}{2\epsilon^2}-V\left(x_j\right)\right)\right]$$

$$=C\int\mathcal{D}x(\tau)\exp\left(\frac{i}{\hbar}\int_0^t Ld\tau\right)$$

Semiclassical Approximation for path integral

$$\varphi\left(x_1,...,x_{N-1}\right)=\epsilon\sum_{j=0}^{N-1}\left(\frac{m}{2}\frac{\left(x_{j+1}-x_j\right)^2}{\epsilon^2}-V\left(x_j\right)\right)$$

$$\frac{\partial\varphi}{\partial x_k}=\epsilon\left(\frac{m}{\epsilon^2}\left(2x_k-x_{k+1}-x_{k-1}\right)-V'\left(x_k\right)\right),\quad\frac{\partial^2\varphi}{\partial x_k\partial x_\ell}=\frac{m}{\epsilon}Q_{k\ell}$$

$$Q_{k\ell}=\begin{pmatrix}2-c_1 & -1 & 0 & 0 & ...\\ -1 & 2-c_2 & -1 & 0 & ...\\ 0 & -1 & 2-c_3 & -1 & ...\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix},\quad c_k=\frac{\epsilon^2}{m}V''\left(x_k\right)$$

$$\lim_{N\to\infty}\varphi(\bar{x})=S\left(x,x_0,t\right)$$

$$D_{k+1}=\left(2-c_{k+1}\right)D_k-D_{k-1}$$

$$m\frac{d^2F(\tau)}{d\tau^2}=-V''(\bar{x}(\tau))F(\tau),\quad F_k=\epsilon D_k$$

$$F(0)=\lim_{\epsilon\to0}\epsilon D_0=\lim_{\epsilon\to0}\epsilon=0,\quad F'(0)=\lim_{\epsilon\to0}\left(D_1-D_0\right)=1.$$

$$F(t) = \frac{\partial x}{\partial v_i} = m\left(\frac{\partial p_i}{\partial x}\right)^{-1} = -m\left(\frac{\partial^2 S}{\partial x_0 \partial x}\right)^{-1}$$

$$K(x, x_0, t) \approx \sum_b \frac{e^{-i\mu_b \pi/2}}{\sqrt{2\pi i\hbar}} \left|\frac{\partial^2 S_b}{\partial x \partial x_0}\right|^{1/2} \exp\left(\frac{i}{\hbar} S_b(x, x_0, t)\right) \quad \text{Van Vleck}$$

(!!! see useful examples in Zhou or later in my theoretical part!)

Типичные примеры

1.2 Matrices, Algebra, Integrals, Functional Analysis, Special Functions

Функан для квантмеха

(!!! тут функан подтягивать нужно, большая тоже работа.)

Об определениях операторов

$$A \text{ Hermitian} \iff A = \overline{A^\top} \iff a_{ij} = \overline{a_{ji}}$$

$$A \text{ Unitary} \iff U^\dagger U = UU^\dagger = I$$

$$\forall \text{ Unitary } U \quad \exists \text{ Unitary } V: \qquad U = V^{-1} D V,$$

$D = \operatorname{diag}\{1, ..., 1\}$

$$\forall \text{ hermitian } A \qquad A = V^{-1} D V$$

V - унитарная матрица, а D - диагональная матрица с вещественными числами.
Например, разложение произвольной унитарной матрицы

$$U = \begin{bmatrix} \cos\rho & -\sin\rho \\ \sin\rho & \cos\rho \end{bmatrix} \begin{bmatrix} e^{i\xi} & 0 \\ 0 & e^{i\zeta} \end{bmatrix} \begin{bmatrix} \cos\sigma & \sin\sigma \\ -\sin\sigma & \cos\sigma \end{bmatrix}$$

О формулах линала для квантмеха

$\operatorname{tr}(\alpha A + \beta B) = \alpha \operatorname{tr} A + \beta \operatorname{tr} B.$
$\operatorname{tr}(AB) = \operatorname{tr}(BA) \qquad \Rightarrow \qquad \operatorname{tr}(C^{-1}AC) = \operatorname{tr} A.$
$\operatorname{tr} A = \operatorname{tr} A^{\mathrm{T}}$
$\ln\det A = \operatorname{tr}\ln A.$
$\operatorname{tr} A \otimes B = (\operatorname{tr} A)(\operatorname{tr} B).$
$\det A_{3\times 3} = \frac{1}{6}\left((\operatorname{tr} A)^3 - 3\operatorname{tr} A \cdot \operatorname{tr} A^2 + 2\operatorname{tr} A^3\right)$

$$\dim\left(\mathcal{H}^A \otimes \mathcal{H}^B\right) = \dim\mathcal{H}^A \cdot \dim\mathcal{H}^B$$
$$\operatorname{tr}(A \otimes B) = \operatorname{tr}(A) \cdot \operatorname{tr}(B)$$
$$(A \otimes B) \cdot (C \otimes D) = (AC) \otimes (BD)$$

Typical integrals for QM

$$\int dx e^{-ax^2/2} = \sqrt{\frac{2\pi}{a}}, \quad \operatorname{Re} a > 0.$$

$$\int dx e^{-ax^2/2} x^2 = \sqrt{\frac{2\pi}{a^3}}.$$

$$\int dx e^{-ax^2/2+bx} = \sqrt{\frac{2\pi}{a}} e^{b^2/2a}.$$

(complex)
$$\int d(\bar{z}, z) e^{-\bar{z}wz} = \frac{\pi}{w}, \quad \operatorname{Re} w > 0$$

$$\int d(\bar{z}, z) e^{-\bar{z}wz+\bar{u}z+\bar{z}v} = \frac{\pi}{w} e^{\bar{u}v/w}, \quad \operatorname{Re} w > 0.$$

$$\int d\mathbf{v} e^{-\mathbf{v}^T A\mathbf{v}/2} = \sqrt{\frac{(2\pi)^N}{\det A}}$$

$$\int d\mathbf{v} \exp\left(-\frac{1}{2}\mathbf{v}^T A\mathbf{v} + \mathbf{j}^T\mathbf{v}\right) = \sqrt{\frac{(2\pi)^N}{\det A}} \exp\left(\frac{1}{2}\mathbf{j}^T A^{-1}\mathbf{j}\right) \qquad \mathbf{v} \to \mathbf{v} + A^{-1}\mathbf{j}$$

(??)

$$\partial_{j_m} e^{\mathbf{j}^T A^{-1}\mathbf{j}/2} = \left(A^{-1}\mathbf{j}\right)_m e^{\mathbf{j}^T A^{-1}\mathbf{j}/2}$$

$$\int d\mathbf{v} e^{-\mathbf{v}^T A\mathbf{v}/2} v_m v_n = \sqrt{\frac{(2\pi)^N}{\det A}} A^{-1}_{mn}$$

$$\langle v_m v_n \rangle = A^{-1}_{mn}$$

$$\langle v_{i_1} \cdots v_{i_{2n}} \rangle = \sum_{\text{pairings}} A^{-1}_{i_{k_1} i_{k_2}} \ldots A^{-1}_{i^{-1}_{k_{2n-1}} i_{k_{2n}}}$$

$$\int d\left(\mathbf{v}^\dagger, \mathbf{v}\right) e^{-\mathbf{v}^\dagger A\mathbf{v}} = \frac{\pi^N}{\det A}$$

$$\int d\left(\mathbf{v}^\dagger, \mathbf{v}\right) e^{-\mathbf{v}^\dagger A\mathbf{v}+\mathbf{w}^\dagger\mathbf{v}+\mathbf{v}^\dagger\mathbf{w}'} = \frac{\pi^N}{\det A} e^{\mathbf{w}^\dagger A^{-1}\mathbf{w}'}$$

$$\langle \bar{v}_{i_1} \cdots \bar{v}_{i_n} v_{j_1} \cdots v_{j_n} \rangle = \sum_{\text{perms}} A^{-1}_{j_1 i_{P_1}} \cdots A^{-1}_{j_n i_{P_n}}$$

Stationary phase approximation

$$\int dx e^{i\varphi(x)/\kappa}$$

$$\int dx e^{i\varphi(x)/\kappa} \approx \sqrt{\frac{2\pi i\kappa}{\varphi''(\bar{x})}} e^{i\varphi(\bar{x})/\kappa} = e^{i\nu\pi/4} \sqrt{\frac{2\pi\kappa}{|\varphi''(\bar{x})|}} e^{i\varphi(\bar{x})/\kappa}, \quad \nu = \operatorname{sign}\left(\varphi''(\bar{x})\right)$$

$$\int d\mathbf{x} e^{i\varphi(\mathbf{x})/\kappa}$$

$$\nabla\varphi = 0$$

$$\int d\mathbf{x} e^{i\varphi(\mathbf{x})/\kappa} = e^{i\nu\pi/4}(2\pi\kappa)^{n/2}\left|\det\frac{\partial^2\varphi(\bar{x})}{\partial x_k \partial x_l}\right|^{-1/2} e^{i\varphi(\bar{x})/\kappa}, \quad \nu = \sum_i \operatorname{sign}(\lambda_i)$$

Typical integrals for scattering

$$\int_{-\infty}^{\infty} e^{-x^2/\beta^2}dx = \beta\sqrt{\pi}; \qquad \int_{-\infty}^{\infty} dx e^{-ax^2} = \sqrt{\frac{\pi}{a}}$$

$$\int_0^{\infty} x^2 \mathrm{e}^{-\gamma x^2}dx = \frac{1}{4\gamma}\sqrt{\frac{\pi}{\gamma}}, \qquad \int_0^{\infty} x^4 e^{-x^2}dx = \frac{3\sqrt{\pi}}{8}$$

$$\int_0^{\infty} \sqrt{x}e^{-x}dx = (1/2)! = \sqrt{\pi}/2$$

$$\int_0^{\infty} x\mathrm{e}^{-\gamma x^2}dx = \frac{1}{2\gamma}, \qquad \int_0^{\infty} x^3\mathrm{e}^{-\gamma x^2}dx = \frac{1}{2\gamma^2}, \qquad \int_0^{\infty} x^5\mathrm{e}^{-\gamma x^2}dx = \frac{1}{\gamma^3}$$

$$\int \frac{e^{-i\mathbf{q}\cdot\mathbf{r}}dV}{|\mathbf{r}+\mathbf{r}_1'-\mathbf{r}_2'|} = \frac{4\pi}{q^2}e^{i\mathbf{q}\cdot(\mathbf{r}_1'-\mathbf{r}_2')}$$

$$\int_0^{\infty} \frac{\sin x}{x^{\nu-1}}dx = \Gamma(2-\nu)\sin\frac{\pi\nu}{2} = -\frac{\pi\sin(\pi\nu/2)}{\Gamma(\nu-1)\sin\pi\nu}.$$

$$\int_{-\infty}^{\infty} \frac{e^{ikx}dk}{k^2-\kappa^2\mp i\varepsilon} = \pm i\frac{\pi}{\kappa}e^{i\pm\kappa|x|}, \qquad \int_{-\infty}^{\infty} \frac{e^{ikx}dk}{k^2+\kappa^2} = \frac{\pi}{\kappa}e^{-\kappa|x|}$$

where x and κ are real, $\kappa > 0$, and $\varepsilon > 0$ is infinitely small. Integrals are calculated using the residue theorem, by closing the integration contour in either the upper ($x > 0$) or lower ($x < 0$) complex half-plane, k.

$$\int \frac{1}{r}e^{i\mathbf{k}\cdot\mathbf{r}-\kappa r}d^3r = \frac{4\pi}{k^2+\kappa^2}, \quad \operatorname{Re}\kappa > 0$$

преобразованиях операторов

(необходимая математика тут)

О типичных преобразованиях операторов

$$[\mathrm{AB},\mathrm{C}] = \mathrm{A}[\mathrm{B},\mathrm{C}] + |\mathrm{A},\mathrm{C}|\mathrm{B}$$
$$|\mathrm{A},\mathrm{BC}| = \mathrm{B}|\mathrm{A},\mathrm{C}| + [\mathrm{A},\mathrm{B}]\mathrm{C}$$

(добавлю еще полезные формулы!)

матричных элементах операторов

(!? тут основная идея. почему такое вообще может быть?)

$$\langle n', L, M-1 \,|A_-|\, nLM\rangle = \sqrt{\frac{(L-M+1)(L+M)}{L(L+1)(2L+1)}}\,\langle n'L\|A\|nL\rangle\,,$$

$$\langle n', L, M-1 \,|A_-|\, n, L-1, M\rangle = \sqrt{\frac{(L-M+1)(L-M)}{L(2L-1)(2L+1)}}\,\langle n'L\|A\|n, L-1\rangle\,,$$

$$\langle n', L-1, M-1 \,|A_-|\, nLM\rangle = -\sqrt{\frac{(L+M-1)(L+M)}{L(2L-1)(2L+1)}}\,\langle n', L-1\|A\|nL\rangle\,.$$

$$\langle n'L'M' \,|A_+|\, nLM\rangle = \langle nLM \,|A_-|\, n'L'M'\rangle^*$$

$$\widehat{\mathbf{A}}\widehat{\mathbf{B}} = \frac{1}{2}\left(\widehat{A}_+\widehat{B}_- + \widehat{A}_-\widehat{B}_+\right) + \widehat{A}_z\widehat{B}_z$$

$$\langle n'LM|\mathbf{AB}|nLM\rangle = \frac{1}{2L+1}\sum_{n'',L''}\langle n'L\|A\|n''L''\rangle\,\langle n''L''\|B\|nL\rangle\,,$$

L'' пробегает значения $L, L\pm 1$.

(абзац про разложение тензоров и усреднение, см. зад. 28 ЛЛ3, пока такое не понял.)

Tensor operators

$|\psi\rangle \to |\psi'\rangle = U(R)|\psi\rangle$

$$A' = U(R)AU(R)^\dagger$$

$\langle\psi'|\,A'\,|\psi'\rangle = \langle\psi|A|\psi\rangle$.

$$\langle\psi'|\,\mathbf{V}\,|\psi'\rangle = R\langle\psi|\mathbf{V}|\psi\rangle$$

$$U(R)V_iU(R)^\dagger = V_jR_{ji}$$

$$[J_i, V_j] = i\hbar\epsilon_{ijk}V_k$$

rank-2 tensor oper

$$U(R)T_{ij}U(R)^\dagger = T_{kl}R_{ki}R_{lj}$$

1.3 Typical Methods

1.3.1 Perturbation theories

Нестационарная теория возмущений в невырожденном случае

$$|\psi(t)\rangle = \sum_n \psi_n(t)|n(t)\rangle, \quad |n(t)\rangle = e^{-iE_nt}|n\rangle$$

$$w_{i\to f} = \left| \int_{-\infty}^{\infty} V_{fi}(t) e^{i\omega_{fi}t} dt \right|^2 \qquad (\hbar = 1)$$

$$i\frac{\partial \psi_n}{\partial t} = \sum_m V_{nm}^{(I)}(t)\psi_m(t), \quad V_{nm}^{(I)} \equiv \langle n(t)|\hat{V}(t)|m(t)\rangle = e^{i\omega_{nm}t}V_{nm}(t), \qquad \omega_{nm} = E_n - E_m.$$

$$c_n^{(0)}(t) = \delta_{ni}$$

$$c_n^{(1)}(t) = \frac{-i}{\hbar}\int_{t_0}^{t} e^{i\omega_{ni}t'} V_{ni}\left(t'\right) dt'$$

$$c_n^{(2)}(t) = \left(\frac{-i}{\hbar}\right)^2 \sum_m \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' e^{i\omega_{nm}t'} V_{nm}\left(t'\right) e^{i\omega_{mi}t''} V_{mi}\left(t''\right), \qquad \omega_{ni} := \frac{E_n - E_i}{\hbar}$$

Proof:

$$\hat{H} = \hat{H}_0 + \lambda V(t)$$

$$\hat{H}_0|i\rangle = E_{\mathrm{i}}^{(0)}|\mathrm{i}\rangle$$

$$|i(t)\rangle_0 = U_0\left(t,t'\right)|i\rangle = e^{-\frac{i}{\hbar}E_1^{(0)}(t-t')}|\mathrm{i}\rangle$$

$$U_0\left(t,t'\right) = e^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0(t-t')}$$

$$U\left(t,t'\right) = \hat{\mathrm{T}}\exp\left\{-\frac{\mathrm{i}}{\hbar}\int_{t'}^{t}\hat{H}(t)dt\right\} \approx \mathbb{1} - \frac{\mathrm{i}}{\hbar}\lambda\int_{t'}^{t} V_I(t)\mathrm{d}t$$

$$|\mathfrak{i}(t)\rangle_I \equiv U_0^{\dagger}\left(t,t'\right)|\mathfrak{i}(t)\rangle := U_I\left(t,t'\right)|i\rangle$$

$$\mathrm{i}\hbar\frac{\partial U_I}{\partial t} = \lambda V_I U_I \qquad V_I := U_0^{\dagger} V U_0$$

(??? строчка, когда нужен второй порядок??? дорешаю ещё задачи!!!)

Вероятность переходов в единицу времени

$$w_{nm} = \frac{2\pi}{\hbar}\left|V_{mn}^{\pm}\right|^2 \delta\left(E_m - E_n \pm \hbar\omega\right) \qquad \text{(золотое правило Ферми)}$$

Работает это для периодических $\widehat{V}(t) = \widehat{V}e^{-i\omega t} + \widehat{V}^{\dagger}e^{i\omega t}$.

$$U(t,t') = \mathbb{1} - \frac{\mathrm{i}}{\hbar}\lambda\int_{t'}^{t} V_I(t)dt$$

$$\langle f\left|U_I(t,t')\right|\mathfrak{i}\rangle \approx -\lambda\frac{\mathrm{i}}{\hbar}\int_{t'}^{t}\langle f\left|V_I(t)\right|\mathfrak{i}\rangle\, dt, \quad |\mathfrak{f}\rangle \neq |\mathfrak{i}\rangle$$

$$\langle f\,|V_I(t)|\,\mathrm{i}\rangle = \left\langle f\left|U_0^\dagger(t,t')\,V(t)U_0(t,t')\right|\mathrm{i}\right\rangle = \langle f|V(t)|\mathrm{i}\rangle e^{\mathrm{i}\omega_{\mathrm{fi}}(t-t')} \qquad \omega_{\mathrm{fi}} = \frac{1}{\hbar}\left(E_{\mathrm{f}}^{(0)} - E_{\mathrm{i}}^{(0)}\right)$$

$$A_{\mathrm{fi}} = -\lambda\frac{\mathrm{i}}{\hbar}\int\limits_{t'}^{t} V_{\mathrm{fi}}(t)e^{\mathrm{i}\omega_{\mathrm{fi}}(t-t')}dt$$

$$W_{\mathrm{i}\to\mathrm{f}} = \frac{1}{\hbar^2}\left|\int\limits_{t'}^{t}\lambda V_{\mathrm{fi}}(t)e^{\mathrm{i}\omega_{\mathrm{fi}}(t-t')}dt\right|^2, \qquad \frac{dW_{\mathrm{i}\to\mathrm{f}}}{d\nu} = \frac{1}{\hbar^2}\left|\int\limits_{t'}^{t}\lambda V_{\mathrm{fi}}(t)e^{\mathrm{i}\omega_{\mathrm{fi}}(t-t')}dt\right|^2$$

Нестационарная теория возмущений в вырожденном случае

(пропишу потом, пока не работал с этим)

Rayleigh–Schrodinger time independent PT for non-degenerate case

$$\hat{H} = \hat{H}_0 + \lambda V, \quad \lambda \to 0 \qquad \hat{H}_0\left|n^{(0)}\right\rangle = E_n^{(0)}\left|n^{(0)}\right\rangle,$$

$|n\rangle = \left|n^{(0)}\right\rangle + \left|n^{(1)}\right\rangle + \ldots, \quad E_n = E_n^{(0)} + E_n^{(1)} + \ldots$

$\left|n^{(p)}\right\rangle = \sum\limits_m c_m^{(p)}\left|m^{(0)}\right\rangle$

$\omega_{nk} := E_n - E_k,$

$$E_n^{(1)} = V_{nn}, \qquad c_{m\neq n}^{(1)} = \frac{V_{mn}}{\omega_{nm}}, \qquad c_n^{(1)} = 0$$

$$E_n^{(2)} = \sum_{k\neq n}\frac{V_{nk}V_{kn}}{\omega_{nm}}, \qquad c_{m\neq n}^{(2)} = \sum_{k\neq n}\frac{V_{mk}V_{kn}}{\omega_{nk}\omega_{nm}} - \frac{V_{nn}V_{mn}}{\omega_{nm}^2}, \qquad c_n^{(2)} = -\frac{1}{2}\sum_k\frac{|V_{nk}|^2}{\omega_{kn}^2}$$

$$E_n^{(3)} = \sum_{m\neq n}\sum_{k\neq n}\frac{V_{nm}V_{mk}V_{kn}}{\omega_{nk}\omega_{nm}} - V_{nn}\sum_{m\neq n}\frac{V_{nm}V_{mn}}{\omega_{nm}^2}$$

Works if: $\qquad \dfrac{|V_{kn}|}{\Delta E_{kn}^{(0)}} \ll 1$

Proof by Landau institute:

$$\hat{H}_0\left|n^{(p)}\right\rangle + \hat{V}\left|n^{(p-1)}\right\rangle = \sum_{l=0}^{p} E_n^{(p-l)}\left|n^{(l)}\right\rangle \qquad \text{(same order)}$$

$\left|n^{(p)}\right\rangle = \sum\limits_i c_i^{(p)}\left|i^{(0)}\right\rangle \quad \Rightarrow \left\langle m^{(0)}\right|,$

$$E_m^{(0)}c_m^{(p)} + \sum_k V_{mk}c_k^{(p-1)} = E_n^{(0)}c_m^{(p)} + \sum_{l=0}^{p-1}E_n^{(p-l)}c_m^{(l)}$$

$$c_{m\neq n}^{(p)} = \frac{1}{\omega_{nm}}\left(\sum_k V_{mk}c_k^{(p-1)} - \sum_{l=0}^{p-1}E_n^{(p-l)}c_m^{(l)}\right)$$

$$m = n \quad \Rightarrow \qquad E_n^{(p)} = \sum_k V_{nk} c_k^{(p-1)} - \sum_{l=1}^{p-1} E_n^{(p-l)} c_n^{(l)}$$

We chose normalization like $\sum_{l=0}^{p} \left\langle n^{(l)} | n^{(p-l)} \right\rangle = 0$ because we want so, then

$$c_n^{(p)} + \left(c_n^{(p)}\right)^* + \sum_{l=1}^{p-1} \left\langle n^{(l)} | n^{(p-l)} \right\rangle = 0 \Rightarrow c_n^{(p)} = -\frac{1}{2} \sum_{l=1}^{p-1} \sum_k c_k^{(l)*} c_k^{(p-l)}$$

All formulas are a particular case (???).

Proof by Kiselev:

$$\left\langle n^{(0)} | n \right\rangle = 1 \qquad \left\langle n^{(0)} | n^{(p)} \right\rangle = 0$$

$$\left(\hat{H}_0 + \lambda V\right) \left\{ \left| n^{(0)} \right\rangle + \sum_{p=1}^{\infty} \lambda^p \left| n^{(p)} \right\rangle \right\} = \left(E_n^{(0)} + \sum_{p=1}^{\infty} \lambda^p \epsilon_p \right) \left\{ \left| n^{(0)} \right\rangle + \sum_{p=1}^{\infty} \lambda^p \left| n^{(p)} \right\rangle \right\}$$

$$\begin{aligned}
\lambda^0: &\quad \hat{H}_0 \left| n^{(0)} \right\rangle &&= E_n^{(0)} \left| n^{(0)} \right\rangle \\
\lambda^1: &\quad \hat{H}_0 \left| n^{(1)} \right\rangle + V \left| n^{(0)} \right\rangle &&= E_n^{(0)} \left| n^{(1)} \right\rangle + \epsilon_1 \left| n^{(0)} \right\rangle \\
&\quad \ldots &&\quad \ldots \\
\lambda^p: &\quad \hat{H}_0 \left| n^{(p)} \right\rangle + V \left| n^{(p-1)} \right\rangle &&= E_n^{(0)} \left| n^{(p)} \right\rangle + \epsilon_1 \left| n^{(p-1)} \right\rangle + \ldots + \epsilon_p \left| n^{(0)} \right\rangle .
\end{aligned}$$

$$\begin{aligned}
\epsilon_1 &= \left\langle n^{(0)} | V | n^{(0)} \right\rangle = V_{nn} \\
\epsilon_2 &= \left\langle n^{(0)} | V | n^{(1)} \right\rangle \\
&\ldots\ldots\ldots \\
\epsilon_p &= \left\langle n^{(0)} | V | n^{(p-1)} \right\rangle \\
\left| n^{(p)} \right\rangle &= \sum_{k \neq n} \left| k^{(0)} \right\rangle \left\langle k^{(0)} | n^{(p)} \right\rangle
\end{aligned}$$

$$\left\langle k^{(0)} | V | n^{(0)} \right\rangle = \left(E_n^{(0)} - E_k^{(0)} \right) \left\langle k^{(0)} | n^{(1)} \right\rangle$$

$$\ldots\ldots\ldots\ldots$$

$$\left\langle k^{(0)} | V | n^{(p-1)} \right\rangle = \left(E_n^{(0)} - E_k^{(0)} \right) \left\langle k^{(0)} | n^{(p)} \right\rangle + \epsilon_1 \left\langle k^{(0)} | n^{(p-1)} \right\rangle + \ldots + \epsilon_{p-1} \left\langle k^{(0)} | n^{(1)} \right\rangle$$

$\epsilon_0 = 0$

$$\left\langle k^{(0)} | n^{(p)} \right\rangle = \frac{1}{E_n^{(0)} - E_k^{(0)}} \left\{ V_{kn}^{(p-1)} - \epsilon_1 \left\langle k^{(0)} | n^{(p-1)} \right\rangle - \ldots - \epsilon_{p-1} \left\langle k^{(0)} | n^{(1)} \right\rangle \right\}$$

$p \geqslant 1, k \neq n, V_{kn}^{(p-1)} = \left\langle k^{(0)} | V | n^{(p-1)} \right\rangle$. From it we see a second-order correction.

Rayleigh–Schrodinger time independent PT for degenerate case

$$\hat{H}_0 \left| n^{(0)}, a \right\rangle = E^{(0)} \left| n^{(0)}, a \right\rangle, \quad a \in (\overline{1,k})$$

$$|n\rangle = \sum_{a=1}^{k} C_a \left| n^{(0)}, a \right\rangle + \sum_{p=1}^{\infty} \lambda^p \left| n^{(p)} \right\rangle$$

$$\det(\hat{V} - \epsilon) = 0 \qquad V_{ba} = \left\langle n^{(0)}, b | V | n^{(0)}, a \right\rangle$$

Proof by Kiselev:

$$\left|\tilde{n}^{(0)}, g\right\rangle, \quad \hat{V}\left|\tilde{n}^{(0)}, g\right\rangle = \epsilon_1^{(g)}\left|\tilde{n}^{(0)}, g\right\rangle,$$

$$\hat{H}_0\left|n^{(p)}, g\right\rangle + V\left|n^{(p-1)}, g\right\rangle = E_n^{(0)}\left|n^{(p)}, g\right\rangle + \epsilon_1^{(g)}\left|n^{(p-1)}, g\right\rangle + \ldots + \epsilon_p^{(g)}\left|n^{(0)}, g\right\rangle$$

Second ordeor of t-indep. RS p.th by inst. Landau: (???)

$$\hat{H}_0\left|n^{(2)}\right\rangle + \hat{V}\left|n^{(1)}\right\rangle = E_n^{(2)}\left|n^{(0)}\right\rangle + E_n^{(1)}\left|n^{(1)}\right\rangle + E_n^{(0)}\left|n^{(2)}\right\rangle$$

$\left\langle n_\alpha^{(0)}\right|$,

$$\sum_{m\neq n,\beta} \frac{V_{\alpha m}V_{m\beta}}{\omega_{nm}} c_{n,\beta}^{(0)} \equiv \sum_\beta H_{\alpha\beta}^{(\text{eff})} c_{n,\beta}^{(0)} = E_n^{(2)} c_{n,\alpha}^{(0)}, \qquad H_{\alpha\beta}^{(\text{eff})} := \sum_{m\neq n} \frac{V_{\alpha m}V_{m\beta}}{\omega_{nm}}$$

$$\det\left(\hat{H}^{(\text{eff})} - E_n^{(2)}\right) = 0$$

$$\hat{H}_0\left|n^{(2)}\right\rangle + \hat{V}\left|n^{(1)}\right\rangle = E_n^{(2)}\left|n^{(0)}\right\rangle + E_n^{(1)}\left|n^{(1)}\right\rangle + E_n^{(0)}\left|n^{(2)}\right\rangle$$

$$\sum_{m\neq n} \frac{V_{\beta m}V_{m\alpha}}{\omega_{nm}} c_{n,\alpha}^{(0)} \equiv \sum_\alpha \hat{H}_{\beta\alpha}^{(\text{eff})} c_{n,\alpha}^{(0)} = E_n^{(2)} c_{n,\beta}^{(0)}, \quad H_{\beta\alpha}^{(\text{eff})} = \sum_{m\neq n} \frac{V_{\beta m}V_{m\alpha}}{\omega_{nm}}$$

Brillouin–Wigner PT for non-degenerate case

$$H = H_0 + \lambda H_1, \qquad \lambda \in [0,1].$$

$$H_0|k\alpha\rangle = \epsilon_k|k\alpha\rangle \qquad \mathcal{H} = \bigoplus \mathcal{H}_k \qquad (\alpha \text{ - for deg.})$$

$$|\psi\rangle: \qquad H|\psi\rangle = E|\psi\rangle.$$

$E = E(\lambda)$, $|\psi\rangle = |\psi\rangle(\lambda)$

$$E = \epsilon_n + \lambda\left\langle n\left|H_1\right|n\right\rangle + \lambda^2 \sum_{k\neq n,\alpha} \frac{\left\langle n\left|H_1\right|k\alpha\right\rangle\left\langle k\alpha\left|H_1\right|n\right\rangle}{\epsilon_n - \epsilon_k} + O\left(\lambda^3\right)$$

$$|\psi\rangle = |n\rangle + \lambda \sum_{k\neq n,\alpha} |k\alpha\rangle \frac{\left\langle k\alpha\left|H_1\right|n\right\rangle}{\epsilon_n - \epsilon_k} + O\left(\lambda^2\right)$$

Proof:

$$P := \sum_\alpha |n\alpha\rangle\langle n\alpha|, \qquad Q := 1 - P.$$

$$(E - H_0)\left|\psi\right\rangle = \lambda H_1|\psi\rangle.$$

$$R := \sum_{k\neq n,\alpha} \frac{|k\alpha\rangle\langle k\alpha|}{E - \epsilon_k}.$$

$$R\left(E - H_0\right) = \left(E - H_0\right)R = Q.$$

$$Q|\psi\rangle = \lambda R H_1|\psi\rangle$$

$$|\psi\rangle = P|\psi\rangle + \lambda R H_1|\psi\rangle.$$

$$|\psi\rangle = \sum_{s\geq 0} \lambda^s \left(RH_1\right)^s P|\psi\rangle.$$

$P|\psi\rangle = |n\rangle$, $\langle n|\psi\rangle = 1$, nondegenerate

$$|\psi\rangle = \sum_{s\geq 0} \lambda^s \left(RH_1\right)^s |n\rangle$$

$$|\psi\rangle = |n\rangle + \lambda \sum_{k\neq n,\alpha} |k\alpha\rangle \frac{\langle k\alpha\,|H_1|\,n\rangle}{E-\epsilon_k} + \lambda^2 \sum_{k\neq n,\alpha} \sum_{k'\neq n,\alpha'} |k\alpha\rangle \frac{\langle k\alpha\,|H_1|\,k'\alpha'\rangle\,\langle k'\alpha'\,|H_1|\,n\rangle}{(E-\epsilon_k)\,(E-\epsilon_{k'})} + \ldots$$

$$0 = \langle n\,|E - H_0 - \lambda H_1|\,\psi\rangle = E - \epsilon_n - \lambda\,\langle n\,|H_1|\,\psi\rangle\,.$$

$$E = \epsilon_n + \lambda\,\langle n\,|H_1|\,n\rangle + \lambda^2\,\langle n\,|H_1 R H_1|\,n\rangle + \lambda^3\,\langle n\,|H_1 R H_1 R H_1|\,n\rangle + \ldots$$

$$E = \epsilon_n + \lambda\,\langle n|H_1|n\rangle + \lambda^2 \sum_{k\neq n,\alpha} \frac{\langle n|H_1|k\alpha\rangle\,\langle k\alpha|H_1|n\rangle}{E-\epsilon_k} + \lambda^3 \sum_{k\neq n,\alpha;k'\neq n,\alpha'} \frac{\langle n|H_1|k\alpha\rangle\,\langle k\alpha|H_1|k'\alpha'\rangle\,\langle k'\alpha'|H_1|n\rangle}{(E-\epsilon_k)\,(E-\epsilon_{k'})} + \ldots$$

$$E = \epsilon_n + \lambda\,\langle n\,|H_1|\,n\rangle + O\left(\lambda^2\right).$$

$$E = \epsilon_n + \lambda\,\langle n\,|H_1|\,n\rangle + \lambda^2 \sum_{k\neq n,\alpha} \frac{\langle n\,|H_1|\,k\alpha\rangle\,\langle k\alpha\,|H_1|\,n\rangle}{\epsilon_n - \epsilon_k} + O\left(\lambda^3\right)$$

$$|\psi\rangle = |n\rangle + \lambda \sum_{k\neq n,\alpha} |k\alpha\rangle \frac{\langle k\alpha\,|H_1|\,n\rangle}{\epsilon_n - \epsilon_k} + O\left(\lambda^2\right)$$

Brillouin–Wigner PT for degenerate case

$$P|\psi\rangle = \sum_{\alpha} |n\alpha\rangle c_\alpha$$

$$0 = \langle n\alpha\,|E - H_0 - \lambda H_1|\,\psi\rangle = (E-\epsilon_n)\,c_\alpha - \lambda\,\langle n\alpha\,|H_1|\,\psi\rangle\,.$$

$$(E-\epsilon_n)\,c_\alpha = \sum_{\beta} \left(\lambda\,\langle n\alpha\,|H_1|\,n\beta\rangle + \lambda^2 \sum_{k\neq n,\gamma} \frac{\langle n\alpha\,|H_1|\,k\gamma\rangle\,\langle k\gamma\,|H_1|\,n\beta\rangle}{E-\epsilon_k} + \ldots \right) c_\beta$$

(??? examples???)

Теория возмущений в частных типичных случаях

Обзор применений и типичных частных случаев нестационарной теории возмущений

Действие возмущения в течение конечного времени.
применяем нестационарную теорию возмущений!
(!?!?!?!)

Постоянное возмущение, $\lambda V(t) = \bar{V}\theta\left(t - t'\right)$:

$$W = \left|\bar{V}_{\text{fi}}\right|^2 \left(\frac{2\sin\left[\omega_{\text{fi}}\left(t - t'\right)/2\right]}{\hbar\omega_{\text{fi}}}\right)^2$$

(добавлю очень известный график про него, см. Киселева пока что)

Периодическое возмущение,

$$\lambda V(t) = \frac{1}{\mathrm{i}}\left\{\bar{V}\mathrm{e}^{\mathrm{i}\omega(t-t')} - \bar{V}^{\dagger}\mathrm{e}^{-\mathrm{i}\omega(t-t')}\right\}, \quad \bar{V}^{\dagger} = \bar{V}, \quad V\left(t'\right) = 0$$

$$\mathrm{d}w_{\text{fi}} = \frac{1}{\hbar}\left|\bar{V}_{\text{fi}}\right|^2 2\pi\delta\left(E_{\text{f}}^{(0)} - E_{\text{i}}^{(0)} + \hbar\omega\right)\mathrm{d}\nu\left(E_{\text{f}}^{(0)}\right) \quad \text{Gold F r}$$

Мгновенное включение возмущения:

$$\lambda V(t) = \bar{V}(s), \quad t = \delta t \cdot s, \quad s \in [0,1].$$

$$\hat{H}(s) = \hat{H}_0 + \bar{V}(s)$$

$$U(\delta t) = \mathbb{1} - \frac{\mathrm{i}}{\hbar}\int_0^1 \hat{H}(s)\delta t\ \mathrm{d}s = \mathbb{1} - \frac{\mathrm{i}}{\hbar}\delta t\bar{H}$$

(это не такая простая задача, в теории подробно пропишу!??!?!)

О типичных тренировочных моделях на теорию возмущений

(особенности, которые лучше помнить - тут.)

Теория возмущений для задач про геометрические деформации (???)

(на полстраницы максимум указаний, скоро прорешаю их уже! обычная теор возмущений, просто пара еще догадок нужны!)

Теория возмущений для задач про линейный отклик (???)

Теория возмущений для энергетических уровней деформированного ядра

О возмущении граничных условий по Мигдалу Крайнову

О внезапных возмущениях по Мигдалу Крайнову

О теории возмущений в случае близких уровней по Мигдалу Крайнову

Частица в периодическом потенциале по МК

Overview of perturbation theories

(??? в чем ее преимущества в сравнении с РШ ТВ???)

(??? а как так вообще, что у нас разные теории возмущений? а третьей еще теории нет??)

(??? как все-таки это связано с ТВ в теормехе?? пока ее в теормехе разбирать буду.)

1.3.2 Green's function methods for QM

(пока в записи по КТП про это, потом сюда допишу в рамках квантмеха и рассеяний!)

Общий формализм пропагаторов

$$|\psi(t)\rangle = \exp\left[\frac{-i\hat{H}\,(t-t_0)}{\hbar}\right]|\psi\,(t_0)\rangle = \sum_a |a\rangle\,\langle a|\psi\,(t_0)\rangle \exp\left[\frac{-iE_a\,(t-t_0)}{\hbar}\right].$$

$$\langle\vec{x}|\psi(t)\rangle = \sum_a \langle\vec{x}|a\rangle \underbrace{\langle a|\psi\,(t_0)\rangle}_{=\int d^3x'\langle a|\vec{x}'\rangle\langle\vec{x}'|\psi(t_0)\rangle.} \exp\left[\frac{-iE_a\,(t-t_0)}{\hbar}\right].$$

$$\psi\,(\vec{x}',t) = \int d^3x K\,(\vec{x}',t;\vec{x},t_0)\,\psi\,(\vec{x},t_0) \qquad K\,(\vec{x}',t;\vec{x},t_0) := \sum_a \langle\vec{x}'|a\rangle\,\langle a|\vec{x}\rangle \exp\left[\frac{-iE_a\,(t-t_0)}{\hbar}\right].$$

$$\lim_{t\to t_0} K\,(\vec{x}',t;\vec{x},t_0) = \delta^3\,(\vec{x}'-\vec{x})\,.$$

$$G(t) \equiv \int d^3x K(x,t;x,0) = \int d^3x \sum_a \langle x|a\rangle\langle a|x\rangle e^{-iE_at/\hbar} = \sum_a \int d^3x \langle a|x\rangle\langle x|a\rangle e^{-iE_at/\hbar} =$$
$$= \sum_a \langle a|a\rangle e^{-iE_at/\hbar} = \sum_a e^{-iE_at/\hbar}.$$

$$Z = \sum_a e^{-\beta E_a} \qquad \beta \equiv 1/(kT) \to -it/\hbar$$

$$\tilde{G}(E) \equiv -\frac{i}{\hbar}\int_0^\infty dt G(t) e^{iEt/\hbar} = -\frac{i}{\hbar}\int_0^\infty dt \sum_a e^{-iE_at/\hbar} e^{iEt/\hbar}. \qquad E \to E + i\varepsilon$$

$$\tilde{G}(E) = \sum_a \frac{1}{E - E_a + i\epsilon}.$$

$$K\,(\vec{x}',t;\vec{x},t_0) = \sum_a \langle\vec{x}'|a\rangle\,\langle a|\vec{x}\rangle \exp\left[\frac{-iE_a\,(t-t_0)}{\hbar}\right] =$$
$$= \sum_a \langle\vec{x}'| \exp\left(-\frac{i\hat{H}t}{\hbar}\right)|a\rangle\langle a| \exp\left(\frac{i\hat{H}t_0}{\hbar}\right)|\vec{x}\rangle = \langle\vec{x}',t|\vec{x},t_0\rangle\,.$$

Examples of propagators

The propagator of a 1D free particle:

$$K\,(x',t;x,t_0) = \left\langle x'\left|e^{-i\hat{H}t/\hbar}\right|x\right\rangle = \int dp\,\langle x'|p\rangle\,e^{-ip^2t/2m\hbar}\langle p|x\rangle =$$
$$= \frac{1}{2\pi\hbar}\int dp \exp\left[\frac{ip\,(x'-x)}{\hbar} - \frac{ip^2\,(t-t_0)}{2m\hbar}\right] =$$
$$= \sqrt{\frac{m}{2\pi i\hbar\,(t-t_0)}} \exp\left[\frac{im\,(x'-x)^2}{2\hbar\,(t-t_0)}\right]\Theta\,(t-t_0)$$

The propagator of a 1D oscillator:

$$K\left(x,x';t\right)=\left(\frac{m\omega}{2\pi i\hbar\sin\omega t}\right)^{\frac{1}{2}}\exp\left(-\frac{m\omega\left(\left(x^2+x'^2\right)\cos\omega t-2xx'\right)}{2i\hbar\sin\omega t}\right)\qquad\text{(Mehler kernel)}$$

(там пара страниц вывода, потом словами укажу его!)

Для уравнения Клейна-Гордона

$$G(x,y)=\frac{1}{(2\pi)^4}\int d^4p\frac{e^{-ip\cdot(x-y)}}{p^2-m^2\pm i\varepsilon}\qquad\qquad p_\mu=(p_0,p),\ p^2=p_\mu p^\mu$$

Для получения решаем $\left(\Box_x+m^2\right)G(x,y)=-\delta(x-y)$, after Fourier transform, $\left(-p^2+m^2\right)G(p)=-1$, and Sokhotski-Plemelj theorem $\frac{1}{x\pm i\varepsilon}=\frac{1}{x}\mp i\pi\delta(x)$ we get (?? додумаю и допишу. тут еще путаница с метрикой, перепишу начало)

Examples of solution by a propagator

(??? write the model!)

$$\Psi(x,t)=\int\limits_0^\infty dx'e^{-\eta x'}\mathcal{K}(t,t_0|x,x')e^{-i\sigma v_F^{(\nu)}kt_0}\chi_{k,\sigma}(x')$$

$$\mathcal{K}(t,t'|x,x')=\sum_{\alpha=\pm}\int\limits_0^\infty dke^{-i\alpha\epsilon_k(t-t')}\Psi_{k,\alpha}(x)\Psi_{k,\alpha}^\dagger(x')+e^{-i\epsilon_e(t-t')}\Psi_e(x)\Psi_e^\dagger(x'),$$

Real-time dynamics in the GF formalism

(??????????????????????)
(см. раздел Галицкого)

Математика для пропагаторов

$$\prod_{n=1}^\infty\left(1-\frac{x^2}{n^2\pi^2}\right)=\frac{\sin x}{x},$$

другом про функцию Грина

О функции Грина в методе интеграла по траекториям

(займусь - пропишу это.)

1.3.3 Scattering, S-matrix, Born Approximation: Main Methods

Elementary scatterings

(I'll solve problems soon!!!)

$$\psi_k^{(+)}(x)=\begin{cases}e^{ikx}+re^{-ikx}, & x\to-\infty\\ te^{ikx}, & x\to+\infty\end{cases},\qquad\psi_k^{(-)}(x)=\begin{cases}t'e^{-ikx}, & x\to-\infty\\ e^{-ikx}+r'e^{ikx}, & x\to+\infty\end{cases}$$

$$\psi^* \Rightarrow \qquad t' = t, \quad r' = -\frac{r^* t}{t^*}$$

$|r| = |r'|$

$$j_{\text{пад}} = \frac{\hbar k}{m}, \qquad j_{\text{отр}} = \frac{\hbar k}{m}|r|^2, \qquad j_{\text{прош}} = \frac{\hbar k}{m}|t|^2$$

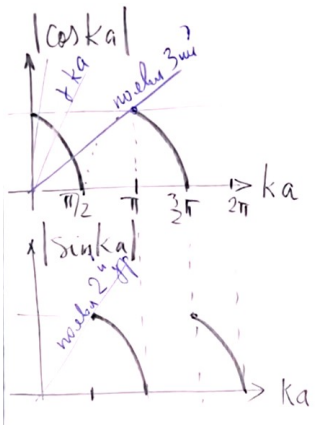
$j(x) = \text{const} \Rightarrow$

$$|r|^2 + |t|^2 = 1$$

$$R := \frac{j_{\text{отр}}}{j_{\text{пад}}} = |r|^2, \qquad T := \frac{j_{\text{прош}}}{j_{\text{пад}}} = |t|^2$$

$$R = |r|^2, \quad T = \frac{k'}{k}|t|^2, \quad R + T = 1$$

(????)



(!! скоро дорешаю, напишу, типичные задачи такого типа в общей физике)

More professional well-known methods

Born approximation

$$\left[-\frac{\hbar^2}{2m}\Delta + U(\mathbf{r})\right]\psi^+_{k_0}(\mathbf{r}) = E\psi^+_{k_0}(\mathbf{r}) \tag{XIII.1}$$

$$\psi^+_{k_0}(\mathbf{r}) \overset{r\to\infty}{\approx} e^{i\mathbf{k}_0 r} + \frac{f(\mathbf{k},\mathbf{k}_0)}{r}e^{ikr}, \quad \mathbf{k} = \frac{k_0\mathbf{r}}{r} \quad U(\mathbf{r}) \downarrow \text{ faster than } \propto 1/r \tag{XIII.2}$$

$k_0 = \sqrt{2mE/\hbar^2}$.
$\sigma = \int |f(\mathbf{k},\mathbf{k}_0)|^2 \, d\Omega_k$.

$$G^+_E(\mathbf{r},\mathbf{r}') = \frac{m}{2\pi\hbar^2|\mathbf{r}-\mathbf{r}'|}e^{ik|\mathbf{r}-\mathbf{r}'|} \tag{XIII.3}$$

$$\psi^+_{\mathbf{k}_0}(\mathbf{r}) = e^{i\mathbf{k}_0\cdot\mathbf{r}} - \frac{m}{2\pi\hbar^2}\int \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}U(\mathbf{r}')\,\psi^+_{\mathbf{k}_0}(\mathbf{r}')\,dV' \tag{XIII.4}$$

$$f(\mathbf{k},\mathbf{k}_0) = -\frac{m}{2\pi\hbar^2}\int e^{-i\mathbf{k}\cdot\mathbf{r}}U(r)\psi^+_{\mathbf{k}_0}(\mathbf{r})dV \tag{XIII.5}$$

First Born approximation:
$\psi^{+}_{\mathbf{k}_0} = e^{i\mathbf{k}_0\cdot\mathbf{r}}$,

$$f^B(\mathbf{q}) = -\frac{m}{2\pi\hbar^2}\tilde{U}(\mathbf{q}), \qquad \tilde{U}(\mathbf{q}) = \int e^{-i\mathbf{q}\cdot\mathbf{r}}U(\mathbf{r})dV \qquad \mathbf{q} := \mathbf{k} - \mathbf{k}_0 \tag{XIII.6}$$

$q_{\text{el}} = 2k\sin(\theta/2)$,

Борновское приближение:

$$\psi^{(1)}(\mathbf{r}) = -\frac{m}{2\pi\hbar^2}\int \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}U(\mathbf{r}')\,e^{i\mathbf{k}\mathbf{r}'}d\mathbf{r}'$$

$$f(\theta,\varphi) \approx -\frac{m}{2\pi\hbar^2}\int e^{-i(\mathbf{k}'-\mathbf{k})\mathbf{r}'}U(\mathbf{r}')\,d\mathbf{r}' \equiv -\frac{m}{2\pi\hbar^2}\tilde{V}_{\mathbf{k}-\mathbf{k}'}$$

$$\hat{T}_E \approx \hat{V}. \qquad \text{Born appr}$$

$\hat{T}_E := \hat{V} + \hat{V}\hat{G}_E^{(0,R)}\hat{V} + \ldots$

$$f_{\text{sp sym, 3D}}(\theta) = -\frac{m}{2\pi\hbar^2}\int d^3\mathbf{r}\; V(\mathbf{r})e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{r}} = -\frac{m}{\hbar^2}\int_0^\infty drr^2V(r)\int_0^\pi e^{-i|\mathbf{k}-\mathbf{k}'|r\cos\varphi}\sin\varphi d\varphi$$

$$= -\frac{2m}{\hbar^2|\mathbf{k}-\mathbf{k}'|}\int_0^\infty drr\sin(|\mathbf{k}-\mathbf{k}'|r)V(r) = -\frac{2m}{2k\hbar^2\sin\frac{\theta}{2}}\int_0^\infty drr\sin\left(2kr\sin\frac{\theta}{2}\right)V(r)$$

valid if:

$$U_0 \ll \frac{\hbar^2}{mR^2} \quad \text{or} \quad U_0 \ll \frac{\hbar v}{R} \tag{XIII.7}$$

In the 1 Born approx. it depends only on the magnitude of momentum transfer, $\hbar q$.

$$\sigma_{3D}(E) = \int |f|^2 d\Omega = 2\pi\int_0^\pi |f|^2\sin\theta d\theta = \frac{\pi\hbar^2}{2mE}\int_0^{8mE/\hbar^2} f^2(q)dq^2 \tag{1}$$

$q := 2k\sin(\theta/2), \qquad \sin\theta d\theta = d(1-\cos\theta) = \frac{d(q^2)}{2k^2}.$

$$f^B_{3D}(q) = -\frac{2m}{\hbar^2 q}\int_0^\infty U(r)\sin(qr)rdr \tag{XIII.8}$$

$\left(k = k_0 = \sqrt{2mE/\hbar^2}\right)$

$$\langle\mathbf{r}|\hat{G}_0|\mathbf{r}'\rangle = \frac{2m}{\hbar^2}\times\begin{cases}\dfrac{1}{2ik}\exp\left(ik\left|x-x'\right|\right), & d=1\\ \dfrac{1}{4i}H_0^+\left(k\left|\mathbf{r}-\mathbf{r}'\right|\right), & d=2\\ -\dfrac{\exp\left(ik\left|\mathbf{r}-\mathbf{r}'\right|\right)}{4\pi\left|\mathbf{r}-\mathbf{r}'\right|}, & d=3\end{cases}$$

$$dN_{\text{pacc}} \equiv d\omega_{i\to f} = 2\pi\left|V_{\boldsymbol{k}-\boldsymbol{k}'}\right|^2\delta\left(\frac{k^2}{2m}-\frac{k^2}{2m}\right)\frac{d^d\boldsymbol{k}'}{(2\pi)^d} = \frac{mk'^{d-2}}{(2\pi)^{d-1}}\left|V_{\boldsymbol{k}-\boldsymbol{k}'}\right|^2\delta\left(k-k'\right)dk'd\Omega$$

Интегрируя по модулю импульса конечных состояний и деля на плотность потока частиц в падающей волне $\boldsymbol{j}_{\text{пад}} = \boldsymbol{k}/m$, получаем:

$$\frac{d\sigma}{d\Omega} = \frac{m^2 k'^{d-3}}{(2\pi)^{d-1}} \left|V_{\boldsymbol{k}-\boldsymbol{k}'}\right|^2$$

(?????)

$d = 3 \quad \Rightarrow \quad d\sigma/d\Omega = m^2 \left|V_{\boldsymbol{k}-\boldsymbol{k}'}\right|^2 / 4\pi^2 \equiv |f(\theta)|^2,$

$|\boldsymbol{k} - \boldsymbol{k}'| = 2k \sin(\theta/2),$

$$f_{\text{sp sym}}(\theta) = -\frac{m}{2\pi} \tilde{V}\left(2k \sin\frac{\theta}{2}\right),$$

Условия применимости Борновского приближения:

$$\frac{m}{\hbar^2 k} \left| \int_0^a \left(1 - e^{2ikr'}\right) U(r')\, dr' \right| \ll 1$$

Slow $\Rightarrow$ $ka \ll 1$, $1 - e^{2ikr'} \approx -2ikr'$,

$$\frac{m}{\hbar^2} \underbrace{\left| \int_0^a r' U(r')\, dr' \right|}_{\sim a^2 U_0} \sim \frac{m U_0 a^2}{\hbar^2} \ll 1 \quad \Leftrightarrow \quad U_0 \ll \frac{\hbar^2}{m a^2},$$

Fast $\Rightarrow$ $ka \gg 1$, $e^{2ikr'} \approx 0$ (oscillates),

$$\frac{m}{\hbar^2 k} \underbrace{\left| \int_0^a U(r')\, dr' \right|}_{\sim a U_0} \sim \frac{m U_0 a}{\hbar^2 k} \quad \Leftrightarrow \quad U_0 \ll \frac{\hbar^2}{m a^2} ka$$

The Born approximation is valid for high energy limit, while the phase shift analysis is useful in the low energy limit

(??? почему? Сузуки так написал)

Partial-wave analysis

For a spherically-symmetric potential,

$$f(k,\theta) = \sum_{l=0}^{\infty} (2l+1) \varphi_l(E) P_l(\cos\theta)$$

$$\varphi_l = \frac{e^{2i\delta_l} - 1}{2ik} = \frac{1}{k(\cot\delta_l - i)} \tag{XIII.9}$$

$$\delta_l(k): \qquad r R_{k,l} \approx C \sin(kr - \pi l/2 + \delta_l),$$

$$\sigma = \sum_{l=0}^{\infty} \sigma_l; \qquad \sigma_l := \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l = \frac{4\pi}{k^2}(2l+1)\left(\cot^2\delta_l + 1\right)^{-1} \tag{XIII.10}$$

$$\operatorname{Im} f(E,\theta=0)=\frac{k}{4\pi}\sigma(E) \tag{XIII.11}$$

1) In the Born approximation ($\left|\delta_l^B\right| \ll 1$),

$$\delta_l^B(k)=-\frac{\pi m}{\hbar^2}\int\limits_0^\infty U(r)J_{l+1/2}^2(kr)rdr \tag{XIII.12}$$

2) In the quasi-classical approximation,

$$\delta_l^{(q)}=\int\limits_{r_0}^\infty\left\{\sqrt{k^2-\frac{2m}{\hbar^2}U(r)-\frac{(l+1/2)^2}{r^2}}-k\right\}dr+\frac{1}{2}\pi\left(l+\frac{1}{2}\right)-kr_0 \tag{XIII.13}$$

r_0 is the turning point of the motion.

$$\delta_{l\ |U(r)|\ll E}^{(q)}\approx-\int\limits_{r_0}^\infty\frac{mU(r)dr}{\hbar^2\sqrt{k^2-(l+1/2)^2/r^2}},\qquad r_0=\frac{(l+1/2)}{k} \tag{XIII.14}$$

A few examples of model scatterings

Example 1: for $V(x)=-V_0\theta(x-a/2)\theta(x+a/2)$

$$r=\frac{(k^2-q^2)\sin(qa)e^{-ika}}{(q^2+k^2)\sin(qa)+2iqk\cos(qa)},\quad t=\frac{2iqke^{-ika}}{(q^2+k^2)\sin(qa)+2iqk\cos(qa)},\quad q^2:=\frac{2mV_0}{\hbar^2}+k^2$$

Well-known special cases of scatterings

Collisions of real particles in a nutshell

(about problems like "neutron hits hydrogen atom, what will come out?")

Slow particles

For the slow particles ($kR\ll 1$), if the potential falls rapidly enough, we plug into

$$f(k,\theta)=\sum_{l=0}^\infty(2l+1)\varphi_l(E)P_l(\cos\theta)\qquad\varphi_l=\frac{e^{2i\delta_l}-1}{2ik}=\frac{1}{k\left(\cot\delta_l-i\right)}$$
$$\sigma=\sum_{l=0}^\infty\sigma_l\qquad\sigma_l=\frac{4\pi}{k^2}(2l+1)\sin^2\delta_l=\frac{4\pi}{k^2}(2l+1)\left(\cot^2\delta_l+1\right)^{-1}$$

the following:

$$k^{2l+1}\cot\delta_l=-\frac{1}{a_l}+\frac{r_lk^2}{2}+\ldots\qquad\text{(eff range expansion)} \tag{XIII.15}$$

a_l - "scattering length"; r_l - "effective interaction range".

If there are no shallow real/virtual (for $l=0$) or quasi-stationary (for $l\neq 0$) levels in the potential, then the second term involving the effective interaction range can be ignored. In this case,

$$\delta_l \approx -a_l k^{2l+1}, \quad |a_l| \leq R^{2l+1}, \quad \text{and} \quad \sigma_l \leq 4\pi(2l+1)(kR)^{4l}R^2$$

The dimensions are $[a_l] = L^{2l+1}, [r_l] = L^{1-2l}$, where L is a unit of length.

On the other hand, if the potential supports a shallow bound state with the energy $|E_l| \ll \hbar^2/mR^2$ and angular momentum, l, the scattering cross-section for the corresponding partial wave, $\sigma_l(E)$, is sharply peaked at $E \approx E_l$ (resonant scattering). Specifically, if a shallow s-level ($l = 0$) exists, then it follows that $|a_0| \gg R$ and

$$\sigma(E) \approx \sigma_{l=0}(E) \approx \frac{2\pi\hbar^2}{m}\frac{1 + r_0\kappa_0}{E + \varepsilon_0} \qquad \begin{array}{r} |E_0| = \varepsilon_0 = \hbar^2\kappa_0^2/2m \\ \kappa_0 = 1/a_0 + r_0/2a_0^2 \end{array} \tag{XIII.16}$$

This is because the poles of the partial-wave amplitude $\varphi_l(E)$ are given by $\cot\delta_l(E) = i$. Combining this with the wave-vector corresponding to a bound state $\kappa = -i\sqrt{2mE/\hbar^2}$ and taking into account $k^{2l+1}\cot\delta_l = -\frac{1}{a_l} + \frac{r_l k^2}{2} + \ldots$ for $a_0 \gg R\,(\approx r_0)$, it follows that $\kappa_0 \approx 1/a_0, \varepsilon_0 \approx \hbar^2/2ma_0^2$ to first order in $1/a_0$. The second-order term is obtained by substituting the first-order term in $k^{2l+1}\cot\delta_l = -\frac{1}{a_l} + \frac{r_l k^2}{2} + \ldots$.

If $a_0 > 0$, it follows that $\kappa_0 > 0$, and ε_0 gives the energy of a real bound state. For $a_0 < 0$, the level is virtual.

For resonant scattering with $l \neq 0$, the behavior of $\sigma_l(E)$ depend crucially on whether the energy level is real or quasi-stationary ($a_l < 0$). In the latter case, $E_l \equiv E_R - i\Gamma_R/2$ (E_R and Γ_R are the level energy and its width), from the poles of the scattering amplitude in the l-th harmonic located at $\cot\delta_l(E_l) = i$, we find:

$$E_R \equiv \frac{\hbar^2 k_R^2}{2m} \approx \frac{\hbar^2}{ma_l r_l} > 0 \qquad\qquad \Gamma_R \approx \left(\frac{2\hbar^2}{m|r_l|}\right) k_R^{2l+1}$$

[308] For a shallow level with $l \neq 0$ to exist, effective interaction range must be negative, $r_l < 0$, so that $E_R, \Gamma_R > 0$ (see Problem 13.44).

$$\sigma_l(E) \approx \frac{(2l+1)\pi}{k_R^2}\frac{\Gamma_R^2}{(E - E_R)^2 + \Gamma_R^2/4} \tag{XIII.17}$$

Fast particles and eikonal approximation

For fast particles ($kR \gg 1$ and $E \gg |U(\mathbf{r})|$), small scattering angles $\theta \leq 1/kR$,

$$f(\mathbf{k}_0, \mathbf{q}_\perp) = \frac{k}{2\pi i}\int [S(\boldsymbol{\rho}) - 1]e^{-i\mathbf{q}_\perp\cdot\boldsymbol{\rho}}d^2\rho \qquad \text{eikonal appr} \tag{XIII.18}$$

$\mathbf{q}_\perp \perp \hbar\mathbf{k}_0, \qquad q_\perp \approx q \approx k\theta;\ q_\parallel \approx k\theta^2/2)$

$$S(\boldsymbol{\rho}) = e^{2i\delta(\boldsymbol{\rho})}, \qquad \delta(\boldsymbol{\rho}) = -\frac{1}{2\hbar v}\int\limits_{-\infty}^{\infty} U(\boldsymbol{\rho}, z)dz \tag{XIII.19}$$

$$\sigma_{\text{tot}}(E) = 2\int [1 - \cos 2\delta(\boldsymbol{\rho})]d^2\rho \tag{XIII.20}$$

$$f_{\text{cntr pot}}(k,\theta) = ik \int\limits_0^\infty \left[1 - e^{2i\delta(\rho)}\right] J_0(k\rho\theta)\rho d\rho \tag{XIII.21}$$

$J_0(z)$ is the 0-order Bessel function.

Other generally important laws of scattering

Derivation of Scattering formalism by Green's function approach

(!! I'll write soon the beginning!)
eq. by Kiselev (!!!)
Lippmann-Schwinger:

$$u^{(\pm)}(\boldsymbol{x},\boldsymbol{k}) = e^{i\boldsymbol{k}\boldsymbol{x}} + \int\limits_{\mathbb{R}^3} G^{(\pm)}(\boldsymbol{x}-\boldsymbol{y},k)\ V(\boldsymbol{y})\ u^{(\pm)}(\boldsymbol{y},\boldsymbol{k})\ d^3\boldsymbol{y}$$

$$G^{(\pm)}(\boldsymbol{x},k) = -\frac{1}{4\pi}\frac{e^{\pm ikr}}{r}$$

For a general case:

$$\chi_{\mathbf{k}}(\mathbf{r}) = \langle\mathbf{r}|\chi\rangle = \langle\mathbf{r}|\hat{G}_E^{(0,R)}\hat{T}_E|\mathbf{k}\rangle = \int d\mathbf{r}'\frac{d\mathbf{k}'}{(2\pi)^d}\langle\mathbf{r}|\hat{G}_E^{(0,R)}|\mathbf{r}'\rangle\langle\mathbf{r}'|\mathbf{k}'\rangle\langle\mathbf{k}'|\hat{T}_E|\mathbf{k}\rangle =$$

$$= \int d\mathbf{r}'\frac{d\mathbf{k}'}{(2\pi)^d}\hat{G}_E^{(0,R)}(\mathbf{r},\mathbf{r}')e^{i\mathbf{k}'\mathbf{r}'}\hat{T}_E(\mathbf{k},\mathbf{k}')$$

$\hat{T}_{E\ \text{brn}} \approx \hat{V}_{\text{brn}}$,

$$\chi_{\mathbf{k}\ \text{brn}}(\mathbf{r}) = \int d\mathbf{r}'\frac{d\mathbf{k}'}{(2\pi)^d}\hat{G}_E^{(0,R)}(\mathbf{r},\mathbf{r}')e^{i\mathbf{k}'\mathbf{r}'}\langle\mathbf{k}'|\hat{V}|\mathbf{k}\rangle$$

(тут конкретно, как связано Борновское приближение и фазы? см. пока задачу Белоусова, пока это додумываю еще.)

О рассеянии тождественных частиц

(допишу пару строчек основной идеи, что имеем зависимость от спина, и используем пространственную четность в.ф. (??))

$$\psi^{(+)}(\boldsymbol{r}) \simeq \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + (-1)^S\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + \frac{\mathrm{e}^{\mathrm{i}\boldsymbol{k}r}}{r}\left\{f(\theta) + (-1)^S f(\pi-\theta)\right\}$$

$$\mathrm{d}\sigma = \left|f(\theta) + (-1)^S f(\pi-\theta)\right|^2\ \mathrm{d}\Omega$$

А для учета еще спина - см. ЛЛ3.137

Например столкновене двух электронов, взаимодействующих по Кулону ($U = e^2/r$), описывается:

$$d\sigma = \left(\frac{e^2}{m_0v^2}\right)\left[\frac{1}{\sin^4(\theta/2)} + \frac{1}{\cos^4(\theta/2)} - \frac{1}{\sin^2(\theta/2)\cos^2(\theta/2)}\cos\left(\frac{e^2}{\hbar v}\ln^2\mathrm{tg}^2\frac{\theta}{2}\right)\right]do$$

$$d\sigma_{e\ll\hbar v} \approx \left(\frac{2e^2}{m_0v^2}\right)^2\frac{4-3\sin^2\theta}{\sin^4\theta}do.$$

(там специфика приближений, см. ЛЛ3.137)

Резонансное рассеяние при малых энергиях

(если притягивающий потенциал и у него уровень вблизи нуля, и особая волна падает, то могут быть приколы. Кому интересно - думайте часа 3 над параграфом Ландау. Специфика, редко такое можно встретить в теории, ну а в экпериментах - не знаю, может, такое и встречается иногда...)

1.3.4 Quasiclassics

Quasiclassics for 1D

$$\psi(x,t) = Ae^{\frac{i}{\hbar}S(x,t)} \quad \Rightarrow \quad \tfrac{1}{2m}\left(\tfrac{\partial S}{\partial x}\right)^2 + U(x) = E \quad \Rightarrow \quad S(x) = \int\limits_{x_0}^{x} p(x)dx, \quad p(x) \equiv \sqrt{2m(E-U(x))}$$

Волновые функции в 1м порядке нарушают унитарность, ведь $j(x) = \hbar p(x)/m$, а в стационарных состояниях этот поток обязан не зависеть от координат. (????) Во 2м порядке:

$$\psi(x) = c_+\psi_+(x) + c_-\psi_-(x)$$

$$\psi_\pm(x) = \frac{e^{\pm i\int\limits_{x_0}^{x} p(x)dx}}{\sqrt{p(x)}}, \qquad \text{(разрешенная о.)}$$

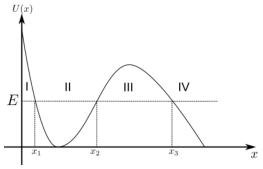
$$\psi_\pm(x) = \frac{e^{\pm\int\limits_{x_0}^{x} |p(x)|dx}}{\sqrt{|p(x)|}}, \quad |p(x)| = \sqrt{2m(U(x)-E)} \qquad \text{(запрещенная о.)}$$

$$\begin{pmatrix} c_+^{(L)} \\ c_-^{(L)} \end{pmatrix} = \hat{A}\begin{pmatrix} c_+^{(R)} \\ c_-^{(R)} \end{pmatrix}, \quad \hat{A} = \begin{pmatrix} e^{-i\pi/4}/2 & e^{i\pi/4} \\ e^{i\pi/4}/2 & e^{-i\pi/4} \end{pmatrix}$$

$$\hat{S}_{\text{cl alwd}} = \begin{pmatrix} e^{-iS} & 0 \\ 0 & e^{iS} \end{pmatrix}, \quad \hat{S}_{\text{cl forb}} = \begin{pmatrix} e^{-S_T} & 0 \\ 0 & e^{S_T} \end{pmatrix}$$

$$\begin{cases} S = \int\limits_{x_1}^{x_2} \sqrt{2m(E-U(x))}dx \\ S_T = \int\limits_{x_2}^{x_3} \sqrt{2m(U(x)-E)}dx \end{cases}$$

Идем из одной крайней области в другую, используя матрицы сшивки A и матриц перехода. Получаем уравнение из условия обнуления растущей экспонент, находим поправку к энергии (или если она мнимая - ширину уровня). Например:



$$\Rightarrow \quad c_I = \underbrace{\hat{A}^\dagger}_{x_1}\underbrace{\hat{S}_{12\text{all}}}_{II}\underbrace{\hat{A}}_{x_2}\underbrace{\hat{S}_{23\text{forb}}}_{III}\underbrace{\hat{A}^\dagger}_{x_3}c_{IV},$$

Критерии применимости:

$$\left|\frac{dp}{dx}\right| \ll p^2 \quad \Leftrightarrow \quad \left|\frac{d\lambda}{dx}\right| \ll 1 \quad \Leftrightarrow \quad m\left|\frac{\partial U/\partial x}{p^3}\right| \ll 1$$

(??????)

ВКБ-приближение пригодно для решения УШ только с аналитическими потенциалами. Однако в ряде случаев для оценки коэффициента подбарьерного прохождения $D(E)$ можно использовать и разрывный потенциал, так как интеграл в показателе экспоненты (ЕК-7.31) нечувствителен к наличию разрывов. Для рассмотрения надбарьерного отражения использование разрывных потенциалов недопустимо.

(абзац про прохождения через барьеры методами ВКБ (!??!?))

Средняя кинетическая энергия стационарного состояния в квазиклассике:

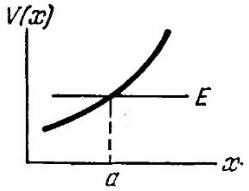
$$\bar{T} = \frac{1}{2}\frac{dE_n}{dn}\left(n + \frac{1}{2}\right).$$

(напишу строчкой, почему, я задачу решал, там подробно вывел это) Кстати, среднюю кинетическую энергию можно выразить через полную с помощью теоремы вириала.

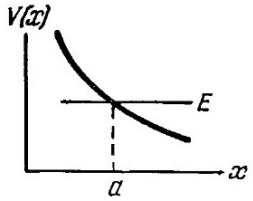
(абзац про обратную задачу)

(мб еще типичные шаблоны про это напишу!!!!)

Квазиклассическое решение справедливо лишь в далекой области от точки поворота ($V(x) = E$).



$$\psi_1 = \begin{cases} \frac{1}{\sqrt{p}} \sin\left(\frac{1}{\hbar}\int\limits_x^a p dx + \frac{\pi}{4}\right) & \text{для } x < a, \\ \frac{1}{2\sqrt{|p|}} e^{-\frac{1}{n}\int\limits_a^x |p| dx} & \text{для } x > a. \end{cases}$$



$$\psi_1 = \begin{cases} \frac{1}{\sqrt{p}} \sin\left(\frac{1}{\hbar}\int\limits_a^x p dx + \frac{\pi}{4}\right) & \text{для } x > a, \\ \frac{1}{2\sqrt{|p|}} e^{-\frac{1}{\hbar}\int\limits_x^a |p| dx} & \text{для } x < a \end{cases}$$

$$\psi = \begin{cases} \frac{1}{\sqrt{p}} e^{\pm\frac{i}{\hbar}\int\limits_x^a p dx} & x < a, \\ \frac{1}{\sqrt{|p|}} e^{\frac{1}{\hbar}\int\limits_a^x |p| dx \mp i\frac{\pi}{4}} + \frac{1}{2\sqrt{|p|}} e^{-\frac{1}{\hbar}\int\limits_a^x |p| dx \pm i\frac{\pi}{4}} & x > a. \end{cases}$$

(дальше у ГК есть еще формулы разные, их потом напишу скорее всего. может, они и не нужны, еще подумаю над задачами)

О правиле Бора-Зоммерфельда (!?!?)

$$\int\limits_{x_1}^{x_2} p(x) dx = \pi\hbar\left(n + \frac{1}{2}\right)$$

Оно получается из (!?!?!!?)

Обсудим дополнительно несколько его свойств.

- Его можно применять только для высоковозбуждённых уровней $n \gg 1$.

- Член 1/2, хоть и мал по сравнению с n - но тем не менее законен; следующие члены разложения будут начинаться с $O(1/n)$. Этот член возник из различных фаз, которые были в задаче сшивки; этот член будет другим для других типов точек остановки. (????) Поэтому часто записывают правило квантования в виде $\pi\hbar(n+\gamma)$ в правой части.

- Номер n тут в точности равен числу нулей квазиклассической волновой функции (которые могут быть только в разрешённой области), то есть полученная волновая функция описывает n-тое возбуждённое состояние.

- Для квантового гармонического осциллятора, правило квантования воспроизводит точный ответ $E = \hbar\omega\left(n+\frac{1}{2}\right)$.

Вид формулы $\oint p(x)dx = 2\pi\hbar\left(n+\frac{1}{2}\right)$ указывает, что номер уровня связан с классическим адиабатическим инвариантом. В частности, сохранения адиабатического инварианта в классической механике и адиабатическая теорема в квантовой механике оказываются связаны посредством этой формулы. (????? почему????)

О типичной математике для квазиклассики

$$\frac{d}{dx}\left(\int\limits_{a(x)}^{b(x)} f(x,t)dt\right) = f(x,b(x))\frac{d}{dx}b(x) - f(x,a(x))\frac{d}{dx}a(x) + \int\limits_{a(x)}^{b(x)}\frac{\partial}{\partial x}f(x,t)dt \quad \text{(Leibniz integr rule)}$$

Часто именно дифференцирование и позволяет сдвинуться.

(тут идея про дифф инт по энергии, вычисление его, потом обратно интегрирования, только так и можно сдвинуться.)

Интегралы часто считаются дифференцированием, а потом заменами переменных. Важно не ошибиться и в переделах интегралов тоже заменять переменные.

(?? мб по тригонометрии пару формул вставлю для этого, пока просто помню, что они очень могут понадобиться)

(можно продифф по n, так получить $\int\limits_a^b \frac{dx}{p}$)

О методе линий Стокса

(см. пока теор части про него, там для ф. Айри и для осциллятора решен он. Мутный метод на самом деле, заумный. Мы выделяем линииб Стокса и анти Стокса, где показатель экспоненты — чисто ещественный, а решения имеют не осциллирующую природу, а экспоненциально возрастающие и затухающие. Дальше у нас какой-то многошаговый обход полюсов и при этом пересечение линий Стокса. Напишу сперва в теории его, потому что место, где я читал про него очень криво его объяснило.)

О поправках к уровням энергии квазиклассикой

(1/2 страницы про такие задачи, тоже типичные формулы тут есть. см. нпр лекции Киселева)

Illustrations of WKB

Oscillator in WKB:

$$\int\limits_{x_{\min}}^{x_{\max}} dx\sqrt{2m\left(E-m^2\omega^2x^2\right)} = \frac{2mE}{m\omega}\frac{\pi}{2} = \left(n+\frac{1}{2}\right)\hbar\pi \qquad \Rightarrow \qquad E = \left(n+\frac{1}{2}\right)\hbar\omega$$

Tunneling through a barrier:

$$\psi(x) = \vec{c}_+^{(II)} e^{\int\limits_{x_2}^{x_1}|p(x)|dx} + \vec{c}_-^{(II)} e^{-\int\limits_{x_2}^{x}|p(x)|dx} \equiv \vec{c}_+^{(II)} e^{-S} e^{\int\limits_{x_1}^{x}|p(x)|dx} + \vec{c}_-^{(II)} e^{S} e^{-\int\limits_{x_1}^{x}|p(x)|dx},$$

$$S = \int\limits_{x_1}^{x_2}|p(x)|dx$$

$$\overleftarrow{c}_{II} = \hat{S}_{12}\vec{c}_{II} = \begin{pmatrix} e^{-S} & 0 \\ 0 & e^{S} \end{pmatrix}\vec{c}_{II}$$

$$c_I = \hat{A}\hat{S}_{12}\hat{A}^\dagger c_{III} = \begin{pmatrix} \frac{e^{-S}}{4} + e^{S} \\ \left(\frac{1}{4}ie^{-S} - ie^{S}\right) \end{pmatrix} t$$

$$\begin{cases} t & \approx e^{-S} \\ r & \approx -i \end{cases} \Rightarrow \begin{cases} T & \approx e^{-2S} \\ R & \approx 1 \end{cases}$$

Гамов

Tunneling out of a Trap:
(картинку Гейгера-Нейтелла добавлю)

$$\psi\left(x_\star\right) = \psi(R)e^{-S/\hbar}$$

$$S = \int\limits_{R}^{x_\star} dx'\sqrt{2m\left(\frac{\alpha}{x'}-E\right)}$$

$$S = \sqrt{\frac{2m}{E}}\pi\alpha = \frac{2\pi\alpha}{\hbar v}$$

$$T = \frac{\left|\psi\left(x_\star\right)\right|^2}{|\psi(R)|^2} = e^{-2S/\hbar}$$

$$v_0 = \sqrt{\frac{2\left(E+V_0\right)}{m}}$$

This means that the particle hits the barrier with frequency $\nu = v_0/R$. The decay rate is then $\Gamma = \nu e^{-2S/\hbar}$ and the lifetime is

$$\tau = \frac{R\sqrt{m}}{\sqrt{2\left(E+V_0\right)}}e^{2S/\hbar}$$

Quarkonium in WKB by Tong:

$$V = Cr$$

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) - \frac{l(l+1)}{r^2}\psi(r)\right) + Cr\psi(r) = E\psi(r)$$

$l = 0$

$\chi = r\psi$

$u = (2mC/\hbar^2)^{1/3}(r - E/C)$

$\chi(u) = \mathrm{Ai}(u)$

$\chi(r = 0) = 0\mathrm{J}$

$$\mathrm{Ai}\left(-\left(\frac{2m}{\hbar^2 C^2}\right)^{1/3} E\right) = 0$$

$y_\star = 2.34, 4.09, 5.52, 6.79, 7.94, 9.02, ...$

$E = (\hbar^2 C^2/2m)^{1/3} y_\star$

других свойствах и случаях применения квазиклассики

(?? Мигдала Крайнова дочитаю - допишу другие указания еще)

(О квазиклассике в черной дыре, как догадаться про это? см. пока Киселева про это)

(О квазиклассике в 2Д и 3Д, что там делать? пока не знаю, в водороде то работает, а вот в других моделях не 1д - видимо, слишком сложный метод, пока не знаю инструкций к нему. в теории пропишу сперва.)

1.3.5 Adiabatic evolution, Berry's connection, f/s variables

Суть нестационарной адиабатики (!?)

$$\hat{H}(t)|n(t)\rangle = E_n(t)|n(t)\rangle$$

$$\omega \ll \Delta E \Rightarrow T \gg 1/\Delta E$$

$$\psi_n(t) \equiv c_n(t) \cdot \exp\left(-i\int\limits_{t_0}^{t} E_n(\tau)d\tau\right),$$

From the sense of $\hat{H}$ one gets that for $m \neq n$ $\quad \langle n(t)\,|\partial_t|\,m(t)\rangle = -\frac{\langle n(t)|\partial_t \hat{H}|m(t)\rangle}{\omega_{nm}(t)}$,

$$c_m(T) \approx \int\limits_{t_0}^{T} \exp\left(i\int\limits_{t_0}^{t} \omega_{mn}(\tau)d\tau\right) \frac{\left\langle m(t)\left|\partial_t \hat{H}\right|n(t)\right\rangle}{\omega_{mn}(t)} dt.$$

(?? допишу чуть лучше вывод!)

Суть стационарной адиабатики, приближения Борна-Опенгеймера, быстрых и медленных переменных (!?)

$$H := \sum_\alpha \frac{\hbar^2}{2M_\alpha}\nabla_\alpha^2 + \sum_i \frac{\hbar^2}{2m}\nabla_i^2 + \frac{e^2}{4\pi\epsilon_0}\left(\sum_{i,j}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_{\alpha,i}\frac{Z_\alpha Z_\beta}{|\mathbf{R}_\alpha - \mathbf{R}_\beta|} - \sum_{i,\alpha}\frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|}\right) \equiv$$

$$\equiv H_{\mathrm{nucl}} + H_{\mathrm{el}}$$

$$H_{\text{nucl}} = -\sum_{\alpha} \frac{\hbar^2}{2M_\alpha}\nabla_\alpha^2 + \frac{e^2}{4\pi\epsilon_0}\sum_{\alpha,i}\frac{Z_\alpha Z_\beta}{|\mathbf{R}_\alpha - \mathbf{R}_\beta|}$$

$$H_{\text{el}} = -\sum_{i} \frac{\hbar^2}{2m}\nabla_i^2 + \frac{e^2}{4\pi\epsilon_0}\left(\sum_{i,j}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} - \sum_{i,\alpha}\frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|}\right)$$

$$H_{\text{el}}\phi_n(\mathbf{r};\mathbf{R}) = \epsilon_n(\mathbf{R})\phi_n(\mathbf{r};\mathbf{R})$$

$$\Psi(\mathbf{r},\mathbf{R}) = \sum_n \Phi_n(\mathbf{R})\phi_n(\mathbf{r};\mathbf{R})$$

$$\left(H_{\text{nucl}} + H_{\text{el}}\right)\Psi = E\Psi$$

$$\sum_n \langle\phi_m| H_{\text{nucl}}\Phi_n |\phi_n\rangle + \epsilon_m(\mathbf{R})\Phi_m = E\Phi_m$$

$$\langle\phi_m| \nabla_{\mathbf{R}}^2\Phi_n |\phi_n\rangle = \sum_k \left(\delta_{mk}\nabla_{\mathbf{R}} + \langle\phi_m| \nabla_{\mathbf{R}} |\phi_k\rangle\right)\left(\delta_{kn}\nabla_{\mathbf{R}} + \langle\phi_k| \nabla_{\mathbf{R}} |\phi_n\rangle\right)\Phi_n$$

$$\sum_{k\neq n}\langle\phi_n| \nabla_{\mathbf{R}} |\phi_k\rangle\langle\phi_k| \nabla_{\mathbf{R}} |\phi_n\rangle = \sum_{k\neq n}\left|\frac{\langle\phi_n| \left(\nabla_{\mathbf{R}} H_{\text{el}}\right)|\phi_k\rangle}{\epsilon_n - \epsilon_k}\right|^2$$

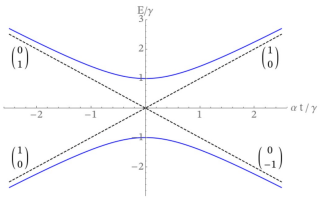
$$H_n^{\text{eff}} = -\sum_\alpha \frac{\hbar^2}{2M_\alpha}\left(\nabla_\alpha - i\mathcal{A}_{n,\alpha}\right)^2 + \frac{e^2}{4\pi\epsilon_0}\sum_{\alpha,i}\frac{Z_\alpha Z_\beta}{|\mathbf{R}_\alpha - \mathbf{R}_\beta|} + \epsilon_n(\mathbf{R})$$

(потом додумаю, в чем польза этих преобразований? см. пока Тонга)

Illustrations of adiabatics

Adiabatics in Landau-Zener:

$$\hat{H}(t) = \begin{pmatrix} \alpha t & \gamma \\ \gamma & -\alpha t \end{pmatrix},$$



$$\alpha t = \gamma\sinh\theta$$

$$E_+(\theta) = \gamma\cosh\theta, \quad |\psi_+(\theta)\rangle = \frac{1}{\sqrt{2\cosh\theta}}\begin{pmatrix} e^{\theta/2} \\ e^{-\theta/2}\end{pmatrix}$$

$$E_-(\theta) = -\gamma\cosh\theta, \quad |\psi_-(\theta)\rangle = \frac{1}{\sqrt{2\cosh\theta}}\begin{pmatrix} e^{-\theta/2} \\ -e^{\theta/2}\end{pmatrix}$$

$$c_+(+\infty) = \int_{-\infty}^{\infty}\exp\left(i\int_0^\theta \omega_{+-}(\theta)\frac{d\tau}{d\theta}d\theta\right)\frac{\langle\psi_+|\partial_\theta\hat{H}|\psi_-\rangle}{\omega_{+-}(\theta)}d\theta$$

$$\partial_\theta\hat{H} = \gamma\begin{pmatrix}\cosh\theta & 0 \\ 0 & -\cosh\theta\end{pmatrix} \Rightarrow \langle\psi_+|\partial_\theta\hat{H}|\psi_-\rangle = \gamma$$

$$\int_0^\theta \omega_{+-}(\theta)\cdot\frac{d\tau}{d\theta}d\theta = \frac{2\gamma^2}{\alpha}\int_0^\theta\cosh^2\theta d\theta = \frac{\gamma^2}{\alpha}\left(\theta + \frac{1}{2}\sinh 2\theta\right)$$

$$c_+(+\infty) \approx \int\limits_{-\infty}^{\infty} \frac{d\theta}{2\cosh\theta} \exp\left(i\frac{\gamma^2}{\alpha}\left(\theta + \frac{1}{2}\sinh 2\theta\right)\right)$$

$f(\theta) = \theta + \frac{1}{2}\sinh 2\theta$;
$f'(\theta) = 1 + \cosh 2\theta \geq 2$,
$z = \theta + \frac{1}{2}\sinh 2\theta \Rightarrow dz = d\theta(1 + \cosh 2\theta) = 2\cosh^2\theta d\theta$,

$$c_+(+\infty) = \int\limits_{-\infty}^{\infty} \frac{\exp\left(i\frac{\gamma^2}{\alpha}z\right)}{4\cosh^3\theta} dz$$

$\cosh\theta = 0 \Rightarrow \theta_k = i\pi(1/2 + k) = z_k$,

$$c_+^{(1)}(+\infty) \sim \exp\left(-\pi\gamma^2/2\alpha\right) \Rightarrow P \sim \exp\left(-\pi\gamma^2/\alpha\right)$$

Adiabatic Spin in a Magnetic Field:

$$H = -\mathbf{B}\cdot\boldsymbol{\sigma} + BM \qquad \mathbf{B} = \begin{pmatrix} B\sin\theta\cos\phi \\ B\sin\theta\sin\phi \\ B\cos\theta \end{pmatrix}$$

$$H = -B\begin{pmatrix} \cos\theta - 1 & e^{-i\phi}\sin\theta \\ e^{+i\phi}\sin\theta & -\cos\theta - 1 \end{pmatrix}$$

$$|\downarrow\rangle = \begin{pmatrix} e^{-i\phi}\sin\theta/2 \\ -\cos\theta/2 \end{pmatrix} \qquad |\uparrow\rangle = \begin{pmatrix} e^{-i\phi}\cos\theta/2 \\ \sin\theta/2 \end{pmatrix}$$

$$\mathcal{A}_\theta = -i\langle\downarrow|\frac{\partial}{\partial\theta}|\downarrow\rangle = 0 \qquad \mathcal{A}_\phi = -i\langle\downarrow|\frac{\partial}{\partial\phi}|\downarrow\rangle = -\sin^2\left(\frac{\theta}{2}\right)$$

$$\mathcal{F}_{\theta\phi} = \frac{\partial\mathcal{A}_\phi}{\partial\theta} - \frac{\partial\mathcal{A}_\theta}{\partial\phi} = -\frac{1}{2}\sin\theta$$

$$\mathcal{F}_{ij}(\mathbf{B}) = -\epsilon_{ijk}\frac{B^k}{2|\mathbf{B}|^3}$$

(?? что тут содержательного мы доказали. ввели свои обозначения, и что?)

Stationary adiabatics in hydrogen:

$$H_{\text{el}} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left[\frac{1}{r} + \frac{1}{|\mathbf{r} - \mathbf{R}|}\right]$$

$$\phi_\pm(\mathbf{r}) = A_\pm\left(\psi_0(\mathbf{r}) \pm \psi_0(\mathbf{r} - \mathbf{R})\right)$$

$$\psi_0 = \sqrt{\frac{1}{\pi a_0^3}}e^{-r/a_0}$$

$E_0 = -e^2/8\pi\epsilon_0 a_0$.

$$A_\pm^2 = \frac{1}{2}\left[1 \pm \int d^3r\psi_0(\mathbf{r})\psi_0(\mathbf{r} - \mathbf{R})\right]^{-1}$$

$$u(R) = \int d^3r \psi_0(\mathbf{r})\psi_0(\mathbf{r}-\mathbf{R}) = \left(1 + \frac{R}{a_0} + \frac{R^2}{3a_0^2}\right) e^{-R/a_0}$$

$$v(R) = \int d^3r \frac{\psi_0(\mathbf{r})\psi_0(\mathbf{r}-\mathbf{R})}{r} = \frac{1}{a_0}\left(1 + \frac{R}{a_0}\right) e^{-R/a_0}$$

$$w(R) = \int d^3r \frac{\psi_0(\mathbf{r})^2}{|\mathbf{r}-\mathbf{R}|} = \frac{1}{R} - \frac{1}{R}\left(1 + \frac{R}{a_0}\right) e^{-2R/a_0}$$

$$\epsilon_\pm(R) = \langle \phi_\pm | H_{\text{el}} | \phi_\pm \rangle = E_0 - 2A_\pm^2(w(R) \pm v(R))$$

$$V_\pm^{\text{eff}}(\mathbf{R}) = \frac{e^2}{4\pi\epsilon_0 R} + \epsilon_\pm(R) = \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{R} - \frac{w(R) \pm v(R)}{1 \pm u(R)}\right) + E_0$$

(??? что получили от этого???)

Adiabatic dynamics in an ellipse:

$$\psi_{N,p}(x,y) = e^{ipx} \cdot \sqrt{\frac{2}{a}} \sin\left(\frac{\pi N}{a}\left(y - \frac{a}{2}\right)\right) \qquad y \in \left(-\frac{a}{2}; \frac{a}{2}\right)$$

$E_{N,p} = \frac{p^2}{2m} + \frac{\pi^2 N^2}{2ma^2}$.

$$\psi_N^{(f)}(y,x) = \sqrt{\frac{2}{a(x)}} \sin\left[\frac{\pi N}{a(x)}\left(y - \frac{a(x)}{2}\right)\right], \quad \varepsilon_N^{(f)}(x) = \frac{\pi^2 N^2}{2ma^2(x)}$$

$$\hat{H}_{\text{eff}}^{(s)} = \frac{\hat{p}_x^2}{2m} + \frac{\pi^2 N^2}{2ma^2(x)}$$

Adiabatic dynamics in a cone:

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1, a \gg b$$

$$E^{(f)} \sim \frac{1}{mb^2},$$

$$\psi_N^{(f)}(y,x) = \frac{1}{\sqrt{y(x)}} \sin\left[\frac{\pi N y}{2y(x)}(y - y(x))\right], \quad \varepsilon_N^{(f)} = \frac{\pi^2 N^2}{8my^2(x)}$$

$$\hat{H}_{\text{eff}} = \frac{\hat{p}_x^2}{2m} + \frac{\pi^2 N^2}{8my^2(x)} = \frac{\hat{p}_x^2}{2m} + \frac{\pi^2 N^2}{8mb^2}\left(1 - \frac{x^2}{a^2}\right)^{-1}$$

$$a \gg b \qquad \Rightarrow \qquad \omega_N = \frac{\pi N}{2mab} \qquad \Rightarrow \qquad E_{N,n} = \frac{\pi^2 N^2}{8mb^2} + \frac{\pi N}{2mab}\left(n + \frac{1}{2}\right)$$

Berry's phase and connection: basics

$$\gamma_n(t) := \int dt \cdot i \left\langle \psi_n(t) | \frac{\partial \psi_n(t)}{\partial t} \right\rangle \qquad - \text{ фаза Берри.}$$

(напомню тут разложение по этим амплитудам с!):

$$c_n(t) = c_n(0) \exp\left(i\gamma_n(t)\right),$$

что легко видеть, переписав $\frac{dc_n(t)}{dt} = ic_n(t) \left\langle \psi_n(t) \left| i\frac{\partial}{\partial t} \right| \psi_n(t) \right\rangle$.

Если гамильтониан зависит не явно от времени, но зависит от какого-то конечного набора параметров $R_i : \hat{H} = \hat{H}(\boldsymbol{R})$, которые, в свою очередь, как-то меняются со временем, то (????)

В свою очередь, мгновенные состояния гамильтониана тоже являются функциями этих параметров $|\psi_n\rangle = |\psi_n(\boldsymbol{R})\rangle$. Тогда выражение для фазы Берри можно переписать:

$$\gamma_n = \int dt \cdot i \langle \psi_n(\boldsymbol{R}) | \nabla_{\boldsymbol{R}} \psi_n(\boldsymbol{R}) \rangle \cdot \frac{\partial \boldsymbol{R}}{\partial t} = \int \boldsymbol{A}_n(\boldsymbol{R}) d\boldsymbol{R}, \quad \boldsymbol{A}_n(\boldsymbol{R}) = i \langle \psi_n(\boldsymbol{R}) | \nabla_{\boldsymbol{R}} \psi_n(\boldsymbol{R}) \rangle$$

$|\widetilde{n}(\boldsymbol{R})\rangle = e^{i\varphi(\boldsymbol{R})} |n(\boldsymbol{R})\rangle \Rightarrow$

$$\widetilde{\boldsymbol{A}}_n(\boldsymbol{R}) = \boldsymbol{A}_n(\boldsymbol{R}) - \nabla_{\boldsymbol{R}} \varphi(\boldsymbol{R}), \quad \widetilde{\gamma}_n = \gamma_n - \varphi(\boldsymbol{R}_f) + \varphi(\boldsymbol{R}_i)$$

Berry's phase and connection: applications and other properties

(????)

1.3.6 Variational Method

Variational method main ideas and formulas

Algorithm:

Main theory for variation by Tong:

Theorem: Consider an arbitrary state $|\psi\rangle$. The expected value of the energy obeys the inequality

$$\langle E \rangle = \langle \psi | H | \psi \rangle \geq E_0$$

(?? idea of proof?)

Now consider a family of states, $|\psi(\alpha)\rangle$, depending on some number of parameters α_i. If we like, we can relax our assumption that the states are normalised and define

$$E(\alpha) = \frac{\langle \psi(\alpha) | H | \psi(\alpha) \rangle}{\langle \psi(\alpha) | \psi(\alpha) \rangle} \qquad \text{Rayleigh-Ritz quotient}$$

$$E(\alpha) \geq E_0 \quad \text{for all } \alpha$$

The most stringent bound on the ground state energy comes from the minimum value of $E(\alpha)$ over the range of α. This, of course, obeys

$$\left. \frac{\partial E}{\partial \alpha_i} \right|_{\alpha = \alpha^\star} = 0$$

giving us the upper bound $E_0 \leq E(\alpha_*)$. This is the essence of the variational method.

Typical examples of variational method

For $H = -\frac{d^2}{dx^2} + x^4$:

$$\psi(x; \alpha) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$

$$E(\alpha) = \sqrt{\frac{\alpha}{\pi}} \int dx \left(\alpha - \alpha^2 x^2 + x^4\right) e^{-\alpha x^2} = \frac{\alpha}{2} + \frac{3}{4\alpha^2}$$

$\alpha_\star^3 = 3,$

$$E(\alpha_\star) \approx 1.08$$

Helium Atom by perturbation theory:

$$H = \frac{\mathbf{p}_1^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0}\frac{1}{r_1} + \frac{\mathbf{p}_2^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0}\frac{1}{r_2} + \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|}$$

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = \psi_{n_1,l_1,m_1}(\mathbf{x}_1)\,\psi_{n_2,l_2,m_2}(\mathbf{x}_2)$$

$$E = -Z^2\left(\frac{1}{n_1^2} + \frac{1}{n_2^2}\right)Ry$$

$$\psi_{1,0,0}(\mathbf{x}) = \sqrt{\frac{Z^3}{\pi a_0^3}}e^{-Zr/a_0} \qquad a_0 := \frac{4\pi\epsilon_0\hbar^2}{me^2} \approx 5\times 10^{-11}\ \mathrm{m}$$

$$\Delta E = \frac{e^2}{4\pi\epsilon_0}\int d^3x_1 d^3x_2 \frac{|\psi_{1,0,0}(\mathbf{x}_1)|^2\,|\psi_{1,0,0}(\mathbf{x}_2)|^2}{|\mathbf{x}_1 - \mathbf{x}_2|}$$

$|\mathbf{x}_1 - \mathbf{x}_2| = \sqrt{(\mathbf{x}_1 - \mathbf{x}_2)^2} = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2\cos\theta_2}$

$$\Delta E = \frac{8\pi^2 e^2}{4\pi\epsilon_0}\left(\frac{Z^3}{\pi a_0^3}\right)^2 \int dr_1 r_1^2 e^{-2Zr_1/a_0}\int dr_2 r_2^2 e^{-2Zr_2/a_0}\int_{-1}^{+1} d(\cos\theta_2)\,\frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2\cos\theta_2}}$$
$$= \frac{5}{8}\frac{Ze^2}{4\pi\epsilon_0 a_0} = \frac{5Z}{4}Ry$$

$$E_0 \approx E + \Delta E = \left(-2Z^2 + \frac{5Z}{4}\right)Ry \approx -74.8\mathrm{eV}$$

$E_{0\mathrm{exact}} \approx -79\mathrm{eV}.$

Helium Atom by variational method:

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = \psi(\mathbf{x}_1)\,\psi(\mathbf{x}_2) \qquad \psi(\mathbf{x};\alpha) = \sqrt{\frac{\alpha^3}{\pi a_0^3}}e^{-\alpha r/a_0}$$

$$E(\alpha) = \int d^3x_1 d^3x_2 \psi^\star(\mathbf{x}_1)\,\psi^\star(\mathbf{x}_2)\,H\psi(\mathbf{x}_1)\,\psi(\mathbf{x}_2)$$

$$H_\alpha = \frac{\mathbf{p}^2}{2m} - \frac{\alpha e^2}{4\pi\epsilon_0}\frac{1}{r}$$

$$H = H_\alpha(\mathbf{p}_1, \mathbf{r}_1) + H_\alpha(\mathbf{p}_2, \mathbf{r}_2) + \frac{e^2}{4\pi\epsilon_0}\left[(\alpha - Z)\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|}\right]$$

$$E(\alpha) = -2\alpha^2 Ry + \frac{e^2}{4\pi\epsilon_0}\left[2(\alpha - Z)\int d^3x\frac{|\psi(\mathbf{x})|^2}{r} + \int d^3x_1 d^3x_2 \frac{|\psi(\mathbf{x}_1)|^2\,|\psi(\mathbf{x}_2)|^2}{|\mathbf{x}_1 - \mathbf{x}_2|}\right]$$

$$\int d^3x \frac{|\psi(\mathbf{x})|^2}{r} = 4\pi \frac{\alpha^3}{\pi a_0^3} \int dr r e^{-2\alpha r/a_0} = \frac{\alpha}{a_0}$$

$$\int d^3x_1 d^3x_2 \frac{|\psi(\mathbf{x}_1)|^2 |\psi(\mathbf{x}_2)|^2}{|\mathbf{x}_1 - \mathbf{x}_2|} = \frac{5\alpha}{8a_0}$$

$$E(\alpha) = \left(-2\alpha^2 + 4(\alpha - Z)\alpha + \frac{5}{4}\alpha\right) Ry$$

$\alpha_\star = Z - 5/16$.

$$E(\alpha_\star) = -2\left(Z - \frac{5}{16}\right)^2 Ry \approx -77.5\text{eV}$$

$E_0 \approx -79.0$eV.

Other about variational method

How Accurate is the Variational Method?

$$|\psi(\alpha_\star)\rangle = \frac{1}{\sqrt{1+\epsilon^2}}(|0\rangle + \epsilon|\phi\rangle)$$

where $|\phi\rangle$ is a normalised state, orthogonal to the ground state, $\langle 0|\phi\rangle = 0$, and ϵ is assumed to be small. Then our guess at the energy is

$$E(\alpha_\star) = \frac{1}{1+\epsilon^2}\left[\langle 0|H|0\rangle + \epsilon(\langle 0|H|\phi\rangle + \langle\phi|H|0\rangle) + \epsilon^2\langle\phi|H|\phi\rangle\right]$$

Importantly the terms linear in ϵ vanish. This is because $\langle\phi|H|0\rangle = E_0\langle\phi|0\rangle = 0$. We can then expand the remaining terms as

$$E(\alpha_\star) = E_0 + \epsilon^2(\langle\phi|H|\phi\rangle - E_0) + \mathcal{O}(\epsilon^2)$$

This means that if the difference from the true ground state is $\mathcal{O}(\epsilon)$, then the difference from the ground state energy is $\mathcal{O}(\epsilon^2)$. This is the reason that the variational method often does quite well.

Existence of bound state by variational Method

(потом додумаю, Тог написал, что запросто это можно устанавливать)

An Example: Existence of bound state of The Yukawa Potential

$$V(r) = -A\frac{e^{-\lambda r}}{r}$$

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$

$$\psi(\mathbf{x};\alpha) = \sqrt{\frac{\alpha^3}{\pi}}e^{-\alpha r}$$

$$E(\alpha) = \frac{\hbar^2\alpha^2}{2m} - \frac{4A\alpha^3}{(\lambda+2\alpha)^2}$$

$$\lambda < \frac{Am}{\hbar^2}$$

Upper Bound on Excited States by variation

(см. Тонга, пока не актуально. можно как-то оценить, ну и хорошо)

1.3.7 Solutions by special functions

General advice for solutions by special functions

I am not sure about this method.

Функции Бесселя $J_m(z), Y_m(z), H_m^{(1,2)}(z), I_m(z), K_m(z)$

$1d:$	e^x	e^{-x}	$\cos x$	$\sin x$	e^{ix}	e^{-ix}
$2d:$	$I_m(x)$	$K_m(x)$	$J_m(x)$	$Y_m(x)$	$H_m^{(1)}(x)$	$H_m^{(2)}(x)$

Функции Инфельда $I_m(z)$ и Макдональда $K_m(z)$

$$\psi''(z) + \frac{1}{z}\psi'(z) - \left(1 + \frac{m^2}{z^2}\right)\psi(z) = 0,$$

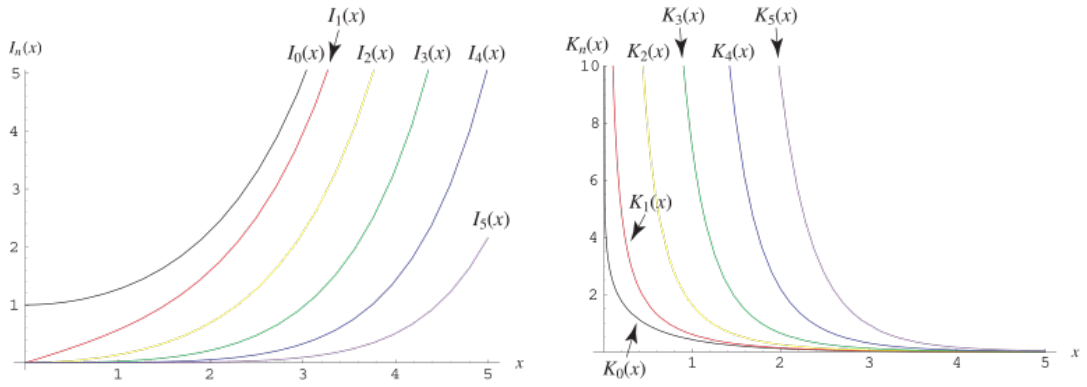
$$\psi(z) = A_1 I_m(z) + A_2 K_m(z)$$

$z \gg 1$ $\qquad I_m(z) \approx \dfrac{1}{\sqrt{2\pi z}} e^z, \qquad K_m(z) \approx \sqrt{\dfrac{\pi}{2z}} e^{-z},$

$z \ll 1$ $\qquad I_m(z) \approx \dfrac{1}{m!}\left(\dfrac{z}{2}\right)^m, \qquad K_m(z) \approx \begin{cases} \frac{(m-1)!}{2}\left(\frac{2}{z}\right)^m, & m \neq 0 \\ \ln\frac{2}{z} - \gamma, & m = 0 \end{cases}, \qquad (\gamma \approx 0.577)$

Функция $K_m(z)$ расходится в нуле, что и должно быть, поскольку W этого уравнения по формуле Лиувилля-Остроградского $\sim 1/x$.

(??)



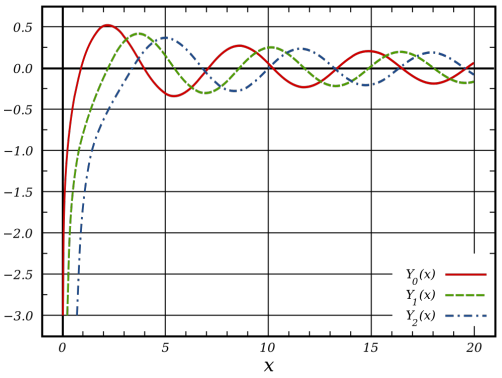
Функции Бесселя $J_m(z)$, Неймана Y_m, Ганкеля $H_m^{(1)}, H_m^{(2)}$

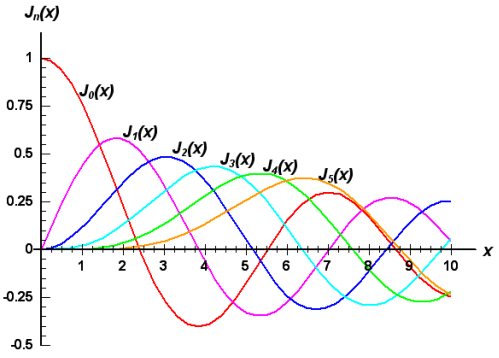
$$\psi''(z) + \frac{1}{z}\psi'(z) + \left(1 - \frac{m^2}{z^2}\right)\psi(z) = 0$$

$$\psi(z) = B_1 J_m(z) + B_2 Y_m(z) \equiv C_1 H_m^{(1)}(z) + C_2 H_m^{(2)}(z)$$

$$z \gg 1: \qquad J_m(z) \approx \sqrt{\frac{2}{\pi z}} \cos\left(z - \frac{m\pi}{2} - \frac{\pi}{4}\right), \quad Y_m(x) \approx \sqrt{\frac{2}{\pi z}} \sin\left(z - \frac{m\pi}{2} - \frac{\pi}{4}\right),$$

$$x \ll 1: \qquad J_m(z) \approx \frac{1}{m!}\left(\frac{z}{2}\right)^m, \quad Y_m(z) \approx \begin{cases} -\frac{(m-1)!}{\pi}\left(\frac{2}{z}\right)^m, & m \neq 0 \\ -\frac{2}{\pi}\left(\ln\frac{2}{z} - \gamma\right), & m = 0 \end{cases},$$





$$H_m^{(1,2)}(x) := J_m(x) \pm iY_m(x).$$

$$H_m^{(1,2)}(z) \approx \sqrt{\frac{2}{\pi z}} e^{\pm i(z - m\pi/2 - \pi/4)}, \qquad z \gg 1$$

$$H_m^{(1,2)}(z) \approx \begin{cases} \mp i\frac{(m-1)!}{\pi}\left(\frac{2}{z}\right)^m, m \neq 0 \\ \mp\frac{2i}{\pi}\left(\ln\frac{2}{z} - \gamma\right) + 1, m = 0 \end{cases} \qquad z \ll 1$$

$$K_m(x) = \frac{\pi}{2} i^{m+1} H_m^{(1)}(ix) = \frac{\pi}{2}(-i)^{m+1} H_m^{(2)}(-ix),$$

$$J_m(ix) = i^m I_m(x)$$

Hypergeometric functions (!!!)

(here def-s, see separate note about them for now)

$${}_1F_1(a, b, z) \approx \frac{\Gamma(b)}{\Gamma(a)} e^z z^{a-b} + \frac{\Gamma(b)}{\Gamma(b-a)}(-z)^{-a}$$

$F(\alpha, \beta, \gamma; z) = (1 - z)^{-\alpha} F\left(\alpha, \gamma - \beta, \gamma; \frac{z}{z-1}\right)$.

Gamma functions (!!!)

Сферические функции

$$Y_{00} = \sqrt{\frac{1}{4\pi}}; \qquad Y_{2,\pm 2} = \sqrt{\frac{15}{32\pi}} \sin^2\theta e^{\pm 2i\phi};$$

$$Y_{1,\pm 1} = \mp\sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm 2i\phi}; \qquad Y^{2,\pm 1} = \mp\sqrt{\frac{15}{8\pi}} \sin\theta\cos\theta e^{\pm 21\phi};$$

$$Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\theta; \qquad Y_{20} = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right).$$

$$\left(1-x^2\right)y''-2xy'+\left[l(l+1)-\frac{m^2}{1-x^2}\right]y=0,$$

$$l=0,1,...; \quad m=0,\pm1,...,\pm l.$$

$$P_l^{|m|}(x)=\frac{1}{2^l l!}\left(1-x^2\right)^{|m|/2}\frac{\mathrm{d}^{l+|m|}}{\mathrm{d}x^{l+|m|}}\left(x^2-1\right)^l. \qquad \text{ф Родрига}$$

$$Y_{lm}(\theta,\varphi)=\sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}P_l^{|m|}(\cos\theta)\mathrm{e}^{\mathrm{i}m\varphi},$$

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}+l(l+1)\right]\Psi(\theta,\varphi)=0;$$

$$\left[\mathrm{i}\frac{\partial}{\partial\varphi}+m\right]\Psi(\theta,\varphi)=0$$

$$\int_0^{2\pi}\mathrm{d}\varphi\int_0^{\pi}Y^*_{l'm'}(\theta,\varphi)Y_{lm}(\theta,\varphi)\sin\theta\mathrm{d}\theta=\delta_{l'l}\delta_{m'm}$$

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y^*_{lm}\left(\theta',\varphi'\right)Y_{lm}(\theta,\varphi)=\delta\left(\cos\theta'-\cos\theta\right)\delta\left(\varphi'-\varphi\right)$$

$$\cos\theta Y_{lm}(\theta,\varphi)=\sqrt{\frac{(l+1)^2-m^2}{(2l+1)(2l+3)}}Y_{l+1,m}(\theta,\varphi)+\sqrt{\frac{l^2-m^2}{(2l-1)(2l+1)}}Y_{l-1,m}(\theta,\varphi),$$

$$Y_{l,-m}=(-1)^mY^*_{lm}$$

$$\left(1-x^2\right)\frac{d^2y}{dx^2}-2x\frac{dy}{dx}+\left[n(n+1)-\frac{m^2}{1-x^2}\right]y=0$$

присоед ф Лежандра: $$P_n^m(x)=\left(1-x^2\right)^{m/2}\left(\frac{d}{dx}\right)^m P_n(x). \qquad m\in Z_+$$

$$\sum_{m'}\langle\hat{\mathbf{r}}|lm'\rangle\langle lm'|U(R)|lm\rangle=\sum_{m'}Y_{lm'}(\hat{\mathbf{r}})D^l_{m'm}(R)$$

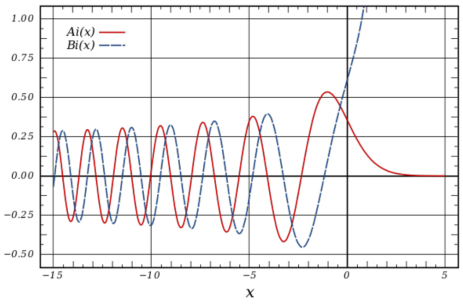
$$Y_{lm}\left(R^{-1}\hat{\mathbf{r}}\right)=\sum_{m'}Y_{lm'}(\hat{\mathbf{r}})D^l_{m'm}(R)$$

$$Y_{lm}(\hat{\mathbf{r}})=\sum_{m'}Y_{lm'}(\hat{\mathbf{z}})D^l_{m'm}\left(R^{-1}\right)$$

Функция Эйри

$$\psi''(z) - z\psi(z) = 0$$
$$\psi(z) = C_1 \operatorname{Ai}(z) + C_2 \operatorname{Bi}(z)$$

$$\operatorname{Ai}(z) \approx \begin{cases} \frac{1}{2\sqrt{\pi}} \frac{1}{z^{1/4}} \exp\left(-\frac{2}{3} z^{3/2}\right), & z \to +\infty \\ \frac{1}{\sqrt{\pi}} \frac{1}{(-z)^{1/4}} \sin\left(\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right), & z \to -\infty \end{cases}$$



Типично ф. Айри решает Шрёдингера с постоянной силой (eg. в $\vec{E}$=const, $U(x) = Fx$):

$$-\frac{\hbar^2}{2m}\psi''(x) + Fx\psi(x) = E\psi(x)$$

$z := \frac{x - E/F}{(\hbar^2/2mF)^{1/3}}$ Решение в классически разрешённой области решения - растущие и затухающие экспоненты.

Функция Эйри возникает естественным образом при выводе граничных условий для квазиклассического приближения (?????).

О свойствах функции Айри на комплексной плоскости и явлении Стокса (???)

Кажется естественным, что асимптотические выражения можно аналитически продолжать за пределы вещественной оси.

Однако, асимптотики не представляются однозначными функциями на комплексной плоскости - для их определения требуется проведение разрезов и выделение ветвей. В то же время сама функция Эйри, разумеется, является однозначной.

Также функция $\operatorname{Ai}(z)$ на $+\infty$ содержит одну экспоненту, а на $-\infty$ -две (в составе синуса), и одно из другого получить аналитическим продолжением невозможно. Всё это связано с так называемым явлением Стокса.

Асимптотики работают только в определённых секторах комплексной плоскости, разделённых лучами (т.н. линиями Стокса), на которых коэффициенты перед компонентами асимптотики (одна компонента содержит $\exp\left(\frac{2}{3}y^{3/2}\right)$, другая $-\exp\left(-\frac{2}{3}y^{3/2}\right)$) меняются скачком.

На этих линиях выражение в экспоненте является вещественным, так что одна из экспонент является максимально убывающей, а другая - максимально растущей.

(мб напишу потом больше, но в записи про спецфункции)

(!!! add plots here!!!!)

комплексный метод перевала

сферических функциях и полиномах Лежандра

$$\int |Y_{lm}|^2 \, do = 1 \qquad do := \sin\theta d\theta d\varphi$$

$$Y_{lm} = \Phi_m(\varphi)\Theta_{lm}(\theta),$$

$\widehat{l}_z\Phi_m(\varphi) := m\Phi_m(\varphi)$.

$$\int_0^{2\pi}\int_0^{\pi} Y^*_{l'm'}Y_{lm}\sin\theta d\theta d\varphi = \delta_{ll'}\delta_{mm'}$$

$$\widehat{\mathbf{l}}^2\psi = \mathbf{l}^2\psi$$

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2} + l(l+1)\psi = 0.$$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta_{lm}}{d\theta}\right) - \frac{m^2}{\sin^2\theta}\Theta_{lm} + l(l+1)\Theta_{lm} = 0.$$

$$\Theta_{lm} = (-1)^m i^l\sqrt{\frac{(2l+1)}{2}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta). \qquad m \geqslant 0$$

$$\Theta_{l,-|m|} := (-1)^m\Theta_{l|m|}, \qquad m < 0$$

$$Y_{ll} = \frac{1}{\sqrt{2\pi}}e^{il\varphi}\Theta_{ll}(\theta)$$

$$\frac{d\Theta_{ll}}{d\theta} - l\operatorname{ctg}\theta\cdot\Theta_{ll} = 0,$$

$$\Theta_{ll} = \text{const}\cdot\sin^l\theta.$$

$$\Theta_{ll} = (-i)^l\sqrt{\frac{(2l+1)!}{2}}\frac{1}{2^l l!}\sin^l\theta$$

$$\langle\mathbf{n}|l,m\rangle = Y_l^m(\theta,\phi) = \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)(l+m)!}{4\pi(l-m)!}}e^{im\phi}\frac{1}{\sin^m\theta}\frac{d^{l-m}}{d(\cos\theta)^{l-m}}(\sin\theta)^{2l} \text{ for } m \geq 0$$

(? абзац пояснений, как не забыть это выражение?)

типичных методах решения УМФ в квантмехе (!?!??!?)

(вот задачи порешаю - пропишу суть этих методов сюда. там много методов умф может быть нужно!)

О методе Лапласа

1.4 Typical Models and Systems

1.4.1 Transitions in atoms, selection rules

(тут также будут указания для задач Овчинкина)

правилах отбора (?)

(скоро порешаю задачи!)

Main selection rules

Для дипольных переходов:

$$\begin{aligned} &\Delta J = \pm 1, 0 && \text{при } J_{\text{нач}} \neq 0 \text{ и } J_{\text{кон}} \neq 0, \\ &\Delta J = \pm 1 && \text{при } J_{\text{нач}} = 0 \text{ или } J_{\text{кон}} = 0. \end{aligned}$$

Отсюда следует, что

$$\Delta m_j = \pm 1, 0$$

Переходы $J_{\text{нач}} = 0 \to J_{\text{кон}} = 0$ запрещены, поскольку в силу поперечности электромагнитных волн не может излучиться фотон с $J = 0$.

Переход с $\Delta J = 0$ при $J_{\text{нач}} \neq 0$ означает поворот вектора $\mathbf{J}$ системы на некий определенный угол.

Отсюда следует, что

$$\Delta \mathbf{S} = 0$$

Переходы с $\Delta L = 0$ невозможны для атомов, в которых испускание света связано с изменением движения всего одного электрона, в частности, для водорода и водородоподобных атомов, а также для атомов с одним электроном сверх заполненных оболочек (т. е. для атомов щелочных металлов).

Этот запрет связан с законом сохранения четности волновой функции.

Emission description from QM

For Hydrogen:

$$I_e \sim \ddot{p_e}^2 \sim \left(\sum e_i r_i\right)^2$$

$$I_\mu \sim \ddot{p_\mu}^2 \sim \left(\frac{1}{2c}\sum e_i \left[r_i v_i\right]\right)^2$$

$I_\mu \sim I_e \left(\frac{v}{c}\right)^2 \approx I_e \cdot 10^{-7}$

Example:

$$|\mathfrak{i}_{\text{at}}\rangle = |L, S; J, M_J\rangle\,, \qquad |\mathfrak{f}_{\text{at}}\rangle = |L', S'; J', M'_J\rangle\,,$$

$$A_{\mathfrak{fi}} = 2\pi\delta\left(\omega_{\mathfrak{fi}} + \omega_{\mathfrak{f}}\right)\omega_{\mathfrak{f}}\boldsymbol{\epsilon}^{*\alpha}_{\lambda_{\mathfrak{f}}}\left(\boldsymbol{k}_{\mathfrak{f}}\right)\langle\mathfrak{f}_{\text{at}}\left|\boldsymbol{d}^{\alpha}\right|\mathfrak{i}_{\text{at}}\rangle\,.$$

$$\boldsymbol{d}^{\alpha}_{\mathfrak{fi}} = \langle\mathfrak{f}_{\text{at}}\left|\boldsymbol{d}^{\alpha}\right|\mathfrak{i}_{\text{at}}\rangle\,.$$

$$\mathrm{d}w_{\mathfrak{fi}} = \frac{\left|A_{\mathfrak{fi}}\right|^2}{T}\frac{\mathrm{d}^3 k_{\mathfrak{f}}}{2\hbar\omega_{\mathfrak{f}}(2\pi)^3} = 2\pi\delta\left(\omega_{\mathfrak{fi}} + \omega_{\mathfrak{f}}\right)\omega_{\mathfrak{f}}^2\frac{\mathrm{d}^3 k_{\mathrm{f}}}{2\hbar\omega_{\mathfrak{f}}(2\pi)^3}\boldsymbol{\epsilon}^{*\alpha}_{\lambda_{\mathfrak{f}}}\boldsymbol{\epsilon}^{\beta}_{\lambda_{\mathfrak{f}}}\boldsymbol{d}^{\alpha}_{\mathfrak{fi}}\boldsymbol{d}^{*\beta}_{\mathfrak{fi}}.$$

$$\sum_{\lambda_{\mathfrak{f}}}\epsilon^{*\alpha}_{\lambda_f}\epsilon^{\beta}_{\lambda_f} = \delta^{\alpha\beta} - n^{\alpha}_{\mathfrak{f}}n^{\beta}_{\mathfrak{f}}, \qquad \boldsymbol{n}_{\mathfrak{f}} = \boldsymbol{k}_{\mathfrak{f}}/k_{\mathfrak{f}}$$

$$\sum_{\lambda_{\mathrm{f}}}\boldsymbol{\epsilon}^{*\alpha}_{\lambda_{\mathrm{f}}}\boldsymbol{\epsilon}^{\beta}_{\lambda_{\mathrm{f}}}\boldsymbol{d}^{\alpha}_{\mathrm{fi}}\boldsymbol{d}^{*\beta}_{\mathrm{fi}} = \boldsymbol{d}_{\mathrm{fi}}\cdot\boldsymbol{d}^{*}_{\mathrm{fi}} - \left(\boldsymbol{d}_{\mathrm{fi}}\cdot\boldsymbol{n}_{\mathfrak{f}}\right)\left(\boldsymbol{d}_{\mathrm{fi}}\cdot\boldsymbol{n}_{\mathfrak{f}}\right)^{*} = \left(\boldsymbol{d}_{\mathrm{fi}}\times\boldsymbol{n}_{\mathrm{f}}\right)\left(\boldsymbol{d}_{\mathrm{fi}}\times\boldsymbol{n}_{\mathrm{f}}\right)^{*} = \left|\boldsymbol{d}_{\mathrm{fi}}\right|^2\sin^2\theta$$

$$\frac{1}{\tau} = \frac{4}{3c^3}\omega_{\mathfrak{f}}^4\left|\tilde{\boldsymbol{d}}_{\mathrm{fi}}\right|^2\frac{1}{\hbar\omega_{\mathrm{f}}}$$

$$\mathcal{J}\left(\omega_{\mathfrak{f}}\right) = \frac{4}{3c^3}\omega_{\mathfrak{f}}^4\left|\tilde{\boldsymbol{d}}_{\mathfrak{fi}}\right|^2.$$

Правила отбора для дипольного момента определяются тремя фактами. Во-первых, согласно теореме Эккарта-Вигнера матричный элемент векторного оператора дипольного момента не равен нулю только в случае, если

$$|\Delta M_J| \leqslant 1, \quad |\Delta J| \leqslant 1, \quad 1 \leqslant J + J'.$$

Отсюда специально отмечаем правило запрета для переходов $0 \to 0'$: матричные элементы с $J = J' = 0$ тождественно равны нулю.

Во-вторых:

$$[S_\alpha, d_\beta] = 0, \quad \left[\boldsymbol{S}^2, d_\alpha\right] = 0,$$

$$\left\langle L', S'; J', M'_J \left| \left[\boldsymbol{S}^2, d_\alpha\right] \right| L, S; J, M_J \right\rangle = \left(S'\,(S'+1) - S(S+1)\right) \langle L', S'; J', M'_J \,|d_\alpha|\, L, S; J, M_J\rangle = 0,$$

поэтому если $\Delta S \neq 0, \quad \Delta M_S \neq 0$, то матричный элемент дипольного момента равен нулю, правило отбора по полному спину имеет вид

$$\Delta S = 0.$$

Далее, правила отбора по четности:

$$P_\mathrm{f} = -P_\mathrm{i}.$$

$$P_\mathrm{atom} = \prod_k (-1)^{l_k} = (-1)^{\sum l_k},$$

l_k - орбитальные моменты электронов в самосогласованном поле. Оно следует из свойства относительно пространственной инверсии $\hat{I}$: $\hat{I}\boldsymbol{d} = -\boldsymbol{d}\hat{I}$. Возьмем матричный элемент этого операторного равенства по конечному и начальному состояниям атома $\langle \mathfrak{f}_\mathrm{at}| \cdot |\mathfrak{i}_\mathrm{at}\rangle$ и учтем, что эти состояния, отвечающие заданным электронным конфигурациям, являются собственными для эрмитова оператора инверсии:

$$\hat{I}\,|\mathfrak{i}_\mathrm{at}\rangle = P_\mathrm{i}\,|\mathfrak{i}_\mathrm{at}\rangle\,, \qquad\qquad \langle \mathfrak{f}_\mathrm{at}|\,\hat{I} = \langle \mathfrak{f}_\mathrm{at}|\,P_\mathrm{f},$$

$$P_\mathfrak{f}\,\langle \mathfrak{f}_\mathrm{at}\,|\boldsymbol{d}|\mathfrak{i}_\mathrm{at}\rangle = -P_\mathrm{i}\,\langle \mathfrak{f}_\mathrm{at}|\boldsymbol{d}|\mathfrak{i}_\mathrm{at}\rangle\,.$$

Значит, матричный элемент дипольного момента не равен нулю, если только пространственные четности вначале и в конце противоположные:

$$P_\mathrm{f} = -P_\mathrm{i},$$

О классификации фотонов и мультипольных волнах (??)

Участвовать в атомных и ядерных процессах может лишь такое электромагнитное излучение, волновая функция которого – собственная функция операторов момента и четности. Плоская волна не имеет определенного момента и четности, однако векторный потенциал такой волны можно разложить в ряд по состояниям с определенными значениями J и P (разложения по мультиполям). Отдельные члены такого разложения будут отвечать электромагнитным волнам (фотонам) с определенными значениями момента и четности, которые могут быть поглощены атомами и ядрами.

Таким образом, задача состоит в том, чтобы перейти от поля фотонов с определенным значением импульса (h/k) к полю фотонов с определенными значениями момента и четности. Прежде чем записать разложение плоской волны по мультиполям, напомним классификацию фотонов по моменту и четности. Полный момент количества движения фотона J принимает целочисленные значения, начиная с единицы: $J = 1, 2, 3, ...$

Полный момент фотона J можно формально рассматривать как векторную сумму спинового S и орбитального L моментов ($\vec{J} = \vec{L} + \vec{S}$), причем орбитальный момент L в данном случае не что иное, как ранг сферических функций YLm, входящих в состав волновой функции фотона.

Фотоны с определенным значением J называются 2J-польными (дипольными, если J = 1; квадрупольными, если J = 2; октупольными, если J = 3 и т.д.).

Для данного J квантовое число орбитального момента L может принимать три значения: L = J+1, J, J–1 так как спин фотона S = 1.

Четность фотона P определяется правилом

$$P = (-1)^{L+1}.$$

(???) Таким образом, фотоны с одинаковым J могут иметь различные значения орбитального момента, а следовательно, и четности.

Фотоны, для которых орбитальный момент совпадает с полным, т. е. L = J, имеют четность $P = (-1)^{J+1}$ и называются магнитными (или кратко MJ) фотонами. Фотоны, для которых $L = J \pm l$, имеют четность $(\breve{}1)^J$ и называются электрическими (или EJ) фотонами.

Фотоны электрического типа, в отличие от фотонов магнитного типа, не имеют определенного значения орбитального момента. Их волновая функция является линейной комбинацией состояний с $L = J \pm 1$. (?????)

$$\mathbf{d} = \sum_i e_i \mathbf{r}_i \qquad \boldsymbol{\mu} = \frac{1}{2c} \sum_i e_i \left[\mathbf{r}_i, \mathbf{v}_i\right]$$

$$I_M = \frac{2\ddot{\mu}^2}{3c^3} \overset{\sim v^2/c^2}{\ll} I_E = \frac{2\,\ddot{\mathrm{d}}^2}{3c^3} \overset{\sim v^2/c^2}{\ll} I_Q = \frac{1}{180c^5} \dddot{Q}^2_{\alpha\beta}.$$

On Wigner–Eckart theorem (?!)

Given a tensor operator $T^{(k)}$ and two states of angular momenta j and j', there exists a constant $\left\langle j \left\| T^{(k)} \right\| j' \right\rangle$ such that for all m, m', and q,

$$\left\langle jm \left| T^{(k)}_q \right| j'm' \right\rangle = \langle j'm'kq|jm\rangle \left\langle j \left\| T^{(k)} \right\| j' \right\rangle,$$

where

- $T^{(k)}_q$ is the q-th component of the spherical tensor operator $T^{(k)}$ of rank k, [2]
- $|jm\rangle$ denotes an eigenstate of total angular momentum J^2 and its z component J_Z,
- $\langle j'm'kq|jm\rangle$ is the Clebsch-Gordan coefficient for coupling j' with k to get j,
- $\left\langle j \left\| T^{(k)} \right\| j' \right\rangle$ denotes [3] some value that does not depend on m, m', nor q and is referred to as the reduced matrix element.

(??? what is the idea of its proof????)

Examples of Wigner–Eckart theorem

Consider the position expectation value $\langle njm|x|njm\rangle$. This matrix element is the expectation value of a Cartesian operator in a spherically symmetric hydrogen-atom-eigenstate basis, which is a nontrivial problem. However, the Wigner-Eckart theorem simplifies the problem. (In fact, we could obtain the solution quickly using parity, although a slightly longer route will be taken.)

We know that x is one component of $\mathbf{r}$, which is a vector. Since vectors are rank-1 spherical tensor operators, it follows that x must be some linear combination of a rank-1 spherical tensor ${T^{(1)}}_q$ with $q \in \{-1, 0, 1\}$. In fact, it can be shown that

$$x = \frac{T^{(1)}_{-1} - T^{(1)}_1}{\sqrt{2}}, \qquad T^{(1)}_q = \sqrt{\frac{4\pi}{3}} r Y^q_1$$

and Y^m_l are spherical harmonics, which themselves are also spherical tensors of rank l. Additionally, ${T^{(1)}}_0 = z$, and

$$T^{(1)}_{\pm 1} = \mp \frac{x \pm iy}{\sqrt{2}}.$$

Therefore,

$$\begin{aligned}\langle njm|x|n'j'm'\rangle &= \left\langle njm \left| \frac{T^{(1)}_{-1} - T^{(1)}_1}{\sqrt{2}} \right| n'j'm' \right\rangle = \\ &= \frac{1}{\sqrt{2}} \left\langle nj \left\| T^{(1)} \right\| n'j' \right\rangle \left(\langle j'm'1(-1)|jm\rangle - \langle j'm'11|jm\rangle \right).\end{aligned}$$

The above expression gives us the matrix element for x in the $|njm\rangle$ basis. To find the expectation value, we set $n' = n, j' = j$, and $m' = m$. The selection rule for m' and m is $m \pm 1 = m'$ for the ${T^{(1)}}_{11}$ spherical tensors. As we have $m' = m$, this makes the ClebschGordan Coefficients zero, leading to the expectation value to be equal to zero.

$$\begin{aligned}\langle \gamma' j'm'| A_q|\gamma jm\rangle &= \langle \gamma' j'| |A\|\gamma j\rangle \langle j'm'|j1mq\rangle \\ \langle \gamma' j'm'| fA_q|\gamma jm\rangle &= \langle \gamma' j'| |fA\|\gamma j\rangle \langle j'm'|j1mq\rangle \\ \langle \gamma' j'm'| f|\gamma jm\rangle &= \delta_{m'm}\delta_{j'j} \langle \gamma' j\|f\|\gamma j\rangle .\end{aligned}$$

$$\langle \gamma' j'| |fA\|\gamma j\rangle = \sum_\Gamma \left\langle \gamma' j'| \|f||\Gamma j' \right\rangle \langle \Gamma j'\|A\|\gamma j\rangle$$

$$\langle \gamma' j'\|\mathbf{A}\cdot\mathbf{B}\|\gamma j\rangle = \sum_{\Gamma j'} \langle \gamma' j\|A\|\Gamma j'\rangle \langle \Gamma j'\|B\|\gamma j\rangle$$

$\mathbf{A}\cdot\mathbf{B} = \sum\limits_q A_q B^\dagger_q$

$$\begin{aligned}\langle \gamma' j'm'| (\mathbf{A}\cdot\mathbf{J}) J_q|\gamma jm\rangle &= \delta_{j'j}\hbar\sqrt{j(j+1)} \langle jm'|j1mq\rangle \langle \gamma' j\|\mathbf{A}\cdot\mathbf{J}\|\gamma j\rangle \\ &= \delta_{j'j}\hbar\sqrt{j(j+1)} \langle jm'|j1mq\rangle \langle \gamma' j\|A\|\gamma j\rangle \langle \gamma j\|J\|\gamma j\rangle \\ &= \delta_{j'j}\hbar^2 j(j+1) \langle jm'|j1mq\rangle \langle \gamma' j\|A\|\gamma j\rangle \\ &= \delta_{j'j}\hbar^2 j(j+1) \langle \gamma' jm'| A_q|\gamma jm\rangle\end{aligned}$$

Об излучении в рамках теории возмущений и взаимодействия с квантовым полем фотонов

$$V_{E1} = -\boldsymbol{d}\cdot\mathcal{E}(t),$$

$\boldsymbol{d} = e\sum\limits_{\text{el}} \boldsymbol{r}_{\text{el}}$.

$$\boldsymbol{\mathcal{E}}(x) = -\partial_0 \mathcal{A}(x) = \mathrm{i}\int \frac{\mathrm{d}^3k}{2(2\pi)^3}\left\{\mathrm{e}^{-\mathrm{i}\omega t}\boldsymbol{\epsilon}_\lambda(\boldsymbol{k})\mathfrak{a}_\lambda(\boldsymbol{k}) - \mathrm{e}^{\mathrm{i}\omega t}\boldsymbol{\epsilon}^*_\lambda(\boldsymbol{k})\mathfrak{a}^\dagger_\lambda(\boldsymbol{k})\right\},$$

$$\left[\mathfrak{a}_\lambda(\boldsymbol{k}), \mathfrak{a}^\dagger_{\lambda'}(\boldsymbol{k}')\right] = 2\hbar\omega(2\pi)^3\delta_{\lambda\lambda'}\delta(\boldsymbol{k}-\boldsymbol{k}'),$$

$$\hat{V}_{E1}(t) = -\mathrm{i}\int \frac{\mathrm{d}^3k}{2(2\pi)^3}\left\{\mathrm{e}^{-\mathrm{i}\omega t}\boldsymbol{d}\cdot\boldsymbol{\epsilon}_\lambda(\boldsymbol{k})\mathfrak{a}_\lambda(\boldsymbol{k}) - \mathrm{e}^{\mathrm{i}\omega t}\boldsymbol{d}\cdot\boldsymbol{\epsilon}^*_\lambda(\boldsymbol{k})\mathfrak{a}^\dagger_\lambda(\boldsymbol{k})\right\}.$$

$$\widehat{\mathbf{V}} = -\frac{e}{mc}\left(\widehat{\mathbf{A}}_{rad}\widehat{\mathbf{p}}\right) + \frac{e^2}{2mc^2}\widehat{\mathbf{A}}^2_{rad} - \mu\left(\widehat{\boldsymbol{\sigma}}\widehat{\mathcal{H}}_{rad}\right),$$

(в кулоновской калибровке), $\widehat{\mathcal{F}}_{\mathrm{rad}} = \mathrm{rot}\,\widehat{\mathbf{A}}_{\mathrm{rad}}$, e, m и μ - электрический заряд, масса и магнитный момент частицы.

Пример: E1-переход 2p → 1s в атоме водорода

$|\mathfrak{i}\rangle = |\,\mathrm{vac}\rangle|2p,m\rangle \quad \mapsto \quad \langle\boldsymbol{r}|\mathfrak{i}\rangle = |\,\mathrm{vac}\rangle\psi_{2p,m}(\boldsymbol{r}) = |\,\mathrm{vac}\rangle R_{2p}(r)y_{1,m}(\theta,\phi).$ $y_{1,\alpha}(\theta,\phi) := \sqrt{\frac{3}{4\pi}}n_\alpha,$

$|\mathfrak{f}\rangle = |\boldsymbol{k}_\mathfrak{f},\lambda_\mathfrak{f}\rangle\,|1s\rangle \quad \mapsto \quad \langle\boldsymbol{r}|\mathfrak{f}\rangle = |\boldsymbol{k}_\mathfrak{f},\lambda_\mathfrak{f}\rangle\frac{1}{\sqrt{4\pi}}R_{1s}(r).$

$$R_{1s}(r) = \frac{2}{\sqrt{a^3}}\mathrm{e}^{-r/a}, \quad R_{2p}(r) = \frac{1}{2\sqrt{6a^5}}r\mathrm{e}^{-r/2a},$$

$$A_{\mathfrak{f}\mathfrak{i}} = -\frac{\mathrm{i}}{\hbar}\int\limits_{-\infty}^{\infty}\mathrm{d}t\mathrm{e}^{\mathrm{i}\omega_{\mathfrak{f}\mathfrak{i}}t}\left\langle\mathfrak{f}\left|\hat{V}_{E1}(t)\right|\mathfrak{i}\right\rangle, \qquad \omega_{\mathfrak{f}\mathfrak{i}} := \frac{1}{\hbar}\{E_{1s}-E_{2p}\} < 0$$

$$\left\langle 1s\left|\boldsymbol{d}^\beta\right|2p,\alpha\right\rangle = \frac{1}{\sqrt{3}}\delta^{\alpha\beta}er_{\mathfrak{f}\mathfrak{i}}.$$

$$\left\langle\boldsymbol{k}_\mathfrak{f},\lambda_\mathfrak{f}\left|\mathfrak{a}^\dagger_\lambda(\boldsymbol{k})\right|\mathrm{vac}\right\rangle = 2\hbar\omega_\mathfrak{f}(2\pi)^3\delta_{\lambda_\mathfrak{f}\lambda}\delta(\boldsymbol{k}_\mathfrak{f}-\boldsymbol{k}).$$

$$\int\frac{\mathrm{d}^3k}{2(2\pi)^3}\boldsymbol{\epsilon}^{*\beta}_\lambda(\boldsymbol{k})\left\langle\boldsymbol{k}_\mathfrak{f},\lambda_\mathfrak{f}\left|\mathfrak{a}^\dagger_\lambda(\boldsymbol{k})\right|\mathrm{vac}\right\rangle = \hbar\omega_\mathfrak{f}\boldsymbol{\epsilon}^{*\beta}_{\lambda_\mathfrak{f}}(\boldsymbol{k}_\mathfrak{f}).$$

$$A_{\mathfrak{f}\mathfrak{i}} = 2\pi\delta(\omega_{\mathfrak{f}\mathfrak{i}}+\omega_\mathfrak{f})\frac{er_{\mathfrak{f}\mathfrak{i}}}{\sqrt{3}}\omega_\mathfrak{f}\epsilon^{*\alpha}_{\lambda_\mathfrak{f}}(\boldsymbol{k}_\mathfrak{f})$$

$$2\pi\delta(\omega)|_{\omega\to0} \mapsto T,$$

$T\to\infty$.

$$\mathrm{d}w_{\mathfrak{f}\mathfrak{i}} = \frac{1}{2l+1}\frac{|A_{\mathfrak{f}\mathfrak{i}}|^2}{T}\frac{\mathrm{d}^3k_\mathfrak{f}}{2\hbar\omega_\mathfrak{f}(2\pi)^3} \overset{\boldsymbol{\epsilon}^*\cdot\boldsymbol{\epsilon}=1}{=} 2\pi\delta(\omega_{\mathfrak{f}\mathfrak{i}}+\omega_\mathfrak{f})\frac{e^2r^2_{\mathfrak{f}\mathfrak{i}}}{9}\omega^2_\mathfrak{f}\frac{\mathrm{d}^3k_\mathfrak{f}}{2\hbar\omega_\mathfrak{f}(2\pi)^3},$$

$$\frac{1}{\tau} := \int\mathrm{d}w_{\mathfrak{f}\mathfrak{i}},$$

$|\boldsymbol{k}_\mathfrak{f}| = \omega_\mathfrak{f}/c, \quad \mathrm{d}^3k_\mathrm{f} = \frac{1}{c^3}\,\mathrm{d}^2\Omega\cdot\omega^2_\mathrm{f}\,\mathrm{d}\omega_\mathrm{f}$

$$\frac{1}{\tau} = \frac{2}{3c^3}\omega^4_\mathrm{f}d^2_{\mathfrak{f}\mathfrak{i}}\frac{1}{\hbar\omega_\mathrm{f}},$$

$$d_{\mathrm{fi}} = \frac{e}{\sqrt{4\pi}} \frac{r_{\mathrm{fi}}}{\sqrt{3}}$$

$$\mathcal{J}_{\mathrm{pol}}\ (\omega_{\mathfrak{f}}) = \frac{\hbar\omega_{\mathfrak{f}}}{\tau} = \frac{2}{3c^3}\omega_{\mathfrak{f}}^4 d_{\mathrm{fi}}^2, \qquad \mathcal{J}\ (\omega_{\mathfrak{f}}) = \frac{4}{3c^3}\omega_{\mathfrak{f}}^4 d_{\mathfrak{fi}}^2.$$

Note:

$$\left\langle f^2(t) \right\rangle = 2\left|f_\omega\right|^2,$$

snice

$$f(t) = f_\omega \mathrm{e}^{-\mathrm{i}\omega t} + f_{-\omega}\mathrm{e}^{\mathrm{i}\omega t}, \quad f_{-\omega} = f_\omega^*,$$

$f^2(t) = 2f_\omega f_{-\omega} + f_\omega^2 \mathrm{e}^{-2\mathrm{i}\omega t} + f_{-\omega}^2 \mathrm{e}^{2\mathrm{i}\omega t}$

$$\Gamma_{2p} = \frac{\hbar}{\tau} = \frac{4}{3c^3}\omega_{\mathfrak{f}}^3 d_{\mathrm{fi}}^2.$$

$$\omega_{\mathrm{fi}} \sim \frac{1}{\hbar} mc^2 \alpha_{\mathrm{em}}^2 \sim 10^{16}\mathrm{c}^{-1}, \quad \hbar\omega_{\mathrm{fi}} \sim 25\text{МэВ},$$

$$d_{\mathrm{fi}} \sim e_0 a \sim \frac{e_0\hbar}{mc\alpha_{\mathrm{em}}},$$

$$\Gamma_{2p} \sim mc^2\alpha_{\mathrm{em}}^5 \ll V_{sl} \sim mc^2\alpha_{\mathrm{em}}^4,$$

$$\Gamma_{2p} = \left(\frac{2}{3}\right)^8 mc^2\alpha_{\mathrm{em}}^5,$$

$$\Gamma_{2p} \approx 4,1 \cdot 10^{-7}\mathrm{eV}, \quad \tau \approx 1,6 \cdot 10^{-9}\mathrm{c},$$

Определение длин волн в линиях мультиплетов

(??? тоже задачи на это есть.)

применениях квантовой теории излучения

(см. Ландау 4, просто обзор всякой специфики КТП)

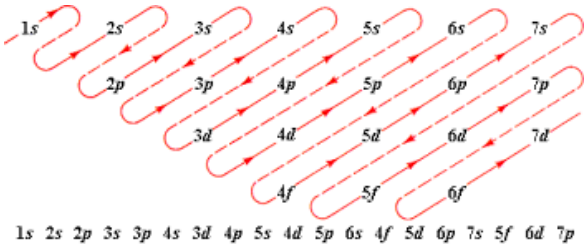
простых задачах на квантовое излучение (!?)

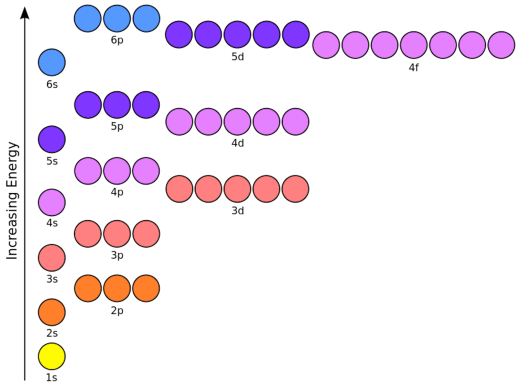
(скоро прорешаю!)
серия Лаймана $0 = R\left(\frac{1}{1^2} - \frac{1}{n^2}\right) \quad (n = 2, 3, 4, ...)$;
серия Пашена $\omega = R\left(\frac{1}{3^2} - \frac{1}{n^2}\right) \quad (n = 4, 5, 6, ...)$;
Еще есть серия Брэкета $\omega = R\left(\frac{1}{4^2} - \frac{1}{n^2}\right) \quad (n = 5, 6, 7, ...)$; и серия Пфунда $\omega = R\left(\frac{1}{5^2} - \frac{1}{n^2}\right) \quad (n = 6, 7, 8, ...)$, и мб другие, но почти никто ими не пользуется.

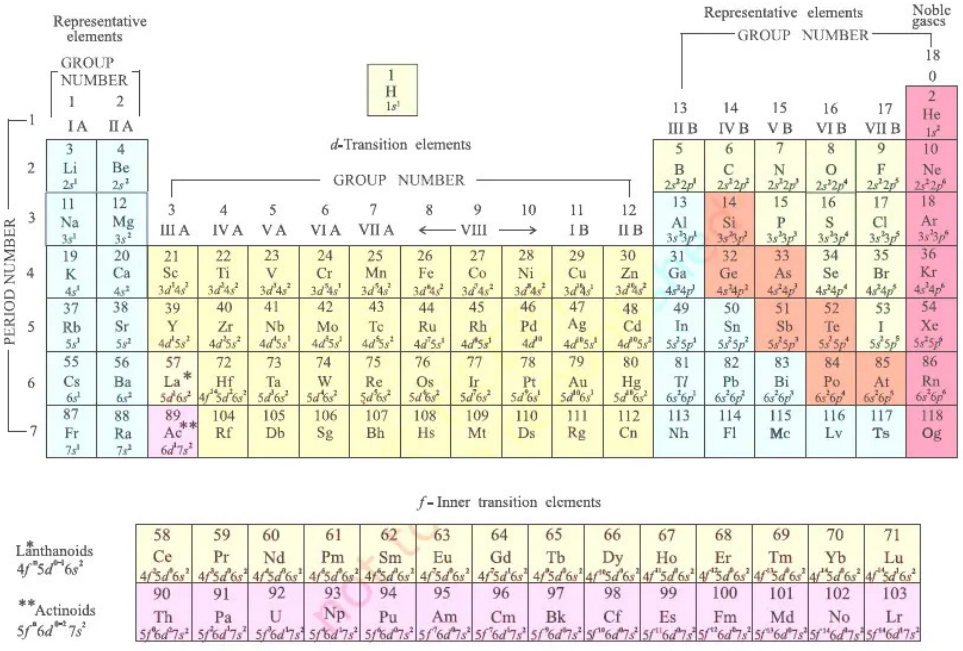
(тут на самом деле про разные задачи, типа такое-то состояние, какое его время жизни? порешаю еще больше их)

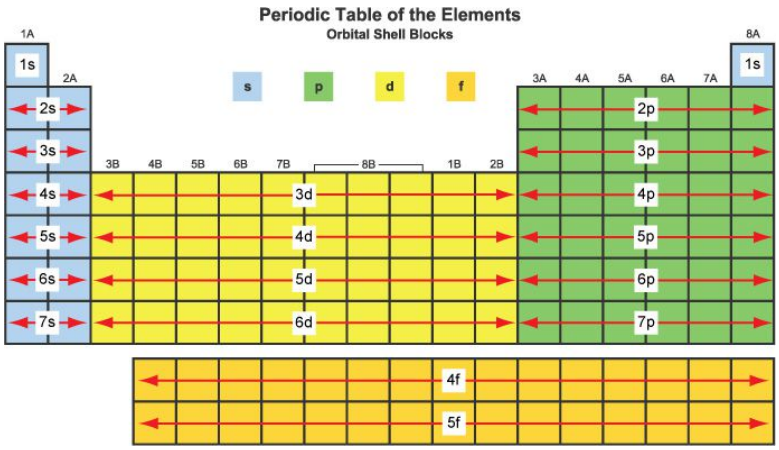
1.4.2 Multi-electron atoms, molecules: basics

Состояния электронов в атоме








Periodic Table of the Elements
Orbital Shell Blocks
1A
8A
2A
3A
4A
5A
6A
7A
3B
4B
5B
6B
7B
8B
1B
2B
s
p
d
f
1s
2s
3s
4s
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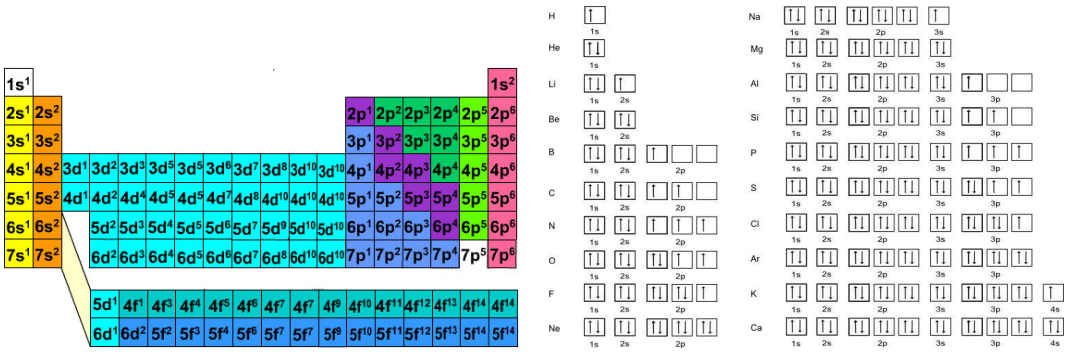
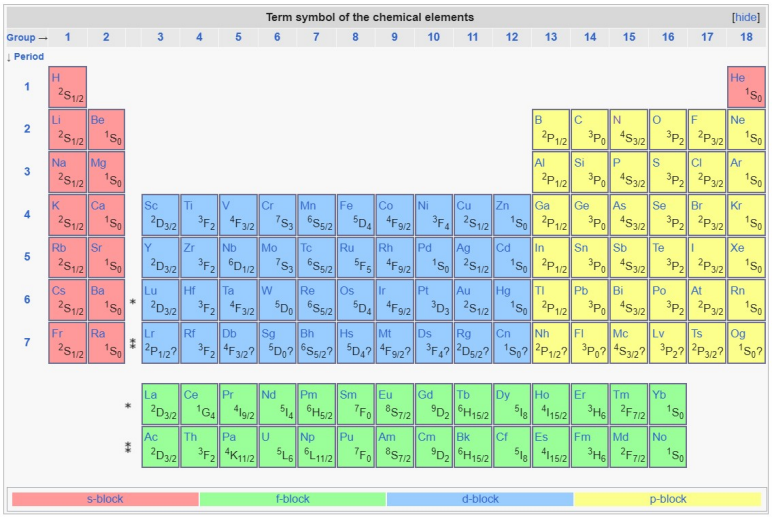
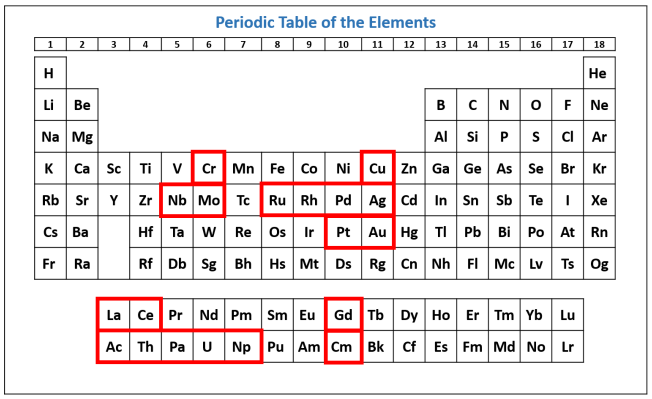
3d
4d
5d
6d
4f
5f




Term symbol of the chemical elements
[hide]
Group →
Period
s-block
f-block
d-block
p-block


Periodic Table of the Elements

Ground-State electronic configurations of exceptions to Madelung's rule:

Cr: $[Ar]3d^5\ 4s$	Rh: $[Kr]4d^8\ 5s$	Gd: $[Xe]4f^7\ 5d\ 6s^2$	Pa: $[Rn]5f^2\ 6d\ 7s^2$
Cu: $[Ar]3d^{10}\ 4s$	Pd: $[Kr]4d^{10}$	Pt: $[Xe]4f^{14}\ 5d^9\ 6s$	U: $[Rn]5f^3\ 6d\ 7s^2$
Nb: $[Kr]4d^4\ 5s$	Ag: $[Kr]4d^{10}\ 5s$	Au: $[Xe]4f^{14}\ 5d^{10}\ 6s$	Np: $[Rn]5f^4\ 6d\ 7s^2$
Mo: $[Kr]4d^5\ 5s$	La: $[Xe]5d\ 6s^2$	Ac: $[Rn]6d\ 7s^2$	Cm: $[Rn]5f^7\ 6d\ 7s^2$
Ru: $[Kr]4d^7\ 5s$	Ce: $[Xe]4f\ 5d\ 6s^2$	Th: $[Rn]6d^2\ 7s^2$	Lr: $[Rn]5f^{14}\ 7s^2\ 7p$

Формализм и типичные свойствах сложных атомов

Смысл и свойства термов

$$^{2S+1}L_J.$$

Определение термов

(??? потренируюсь на задачах, именно этот параграф и для задач такого типа!)

Первое правило Хунда: в первом порядке ТВ энергия атома имеет минимальное значения в состояниях с максимально возможным значением полного спина S. Если при этом возможны несколько различных значений полного орбитального момента, минимальную энергию имеют состояния с максимальным значением L.

Второе правило Хунда (о влиянии тонкого расщепления): во втором порядке ТВ минимальную энергию имеет терм с $J = |L - S|$, если электронная оболочка заполнена меньше, чем наполовину, и с $J = L + S$, если она заполнена на половину или более.

(!!! порешаю задачи!!!)

(??? почему исключения бывают??)

Определитель Слэтера

$$\Psi^F_{n_1,n_2,...,n_N}(\xi_1,\xi_2,...,\xi_N) = \frac{1}{\sqrt{N!}}\det\begin{pmatrix} \psi_{n_1}(\xi_1) & \psi_{n_2}(\xi_1) & ... & \psi_{n_N}(\xi_1) \\ \psi_{n_1}(\xi_2) & \psi_{n_2}(\xi_2) & ... & \psi_{n_N}(\xi_2) \\ \vdots & & & \vdots \\ \psi_{n_1}(\xi_N) & \psi_{n_2}(\xi_N) & ... & \psi_{n_N}(\xi_N) \end{pmatrix} \qquad \xi := \{\boldsymbol{r}, m_s\},$$

Это общий вид антисимметричной суммы произведения одночастичных волновых функций каждого электрона.

Для двух невзаимодействующих нерелятивистских частиц спиновые и координатные переменные разделяются, при этом формальное выражение имеет одинаковый вид для ферми- и бозе-частиц:

$$\Psi^F_{n_1,n_2}(\xi_1,\xi_2) = \sum_{S,M_S} C_{S,M_S}\Phi^{(S)}_{n_1,n_2}(\mathbf{r}_1,\mathbf{r}_2)\,\lambda(S,M_S).$$

$$\Phi^{(S)}_{n_1,n_2}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}\left(\psi_{n_1}(\mathbf{r}_1)\psi_{n_2}(\mathbf{r}_2) + (-1)^S\psi_{n_1}(\mathbf{r}_2)\psi_{n_2}(\mathbf{r}_1)\right).$$

Здесь $n_{1,2}$ - полный набор квантовых чисел одночастичных состояний (без учета спина), $\chi(S,M_S)$ - спиновая функция, описывающая состояние с определенным значением суммарного спина двух частиц S.

Приближение Хартри-Фока

Уравнения Хартри моделируют экранирование потенциальной энергии электрона «облаком» другого.

Уравнения Хартри–Фока по Zhou

Уравнения Хартри–Фока по Киселеву

(не уверен, что это хорошо объяснено тут, потом додумаю)

$$E_A\psi_A = \left\{-\frac{1}{2}\triangle_A - \frac{Z}{r_A} + \phi_B(\boldsymbol{r}_A)\right\}\psi_A,$$
$$E_B\psi_B = \left\{-\frac{1}{2}\triangle_B - \frac{Z}{r_B} + \phi_A(\boldsymbol{r}_B)\right\}\psi_B,$$
$$\phi_B(\boldsymbol{r}_A) = \int \mathrm{d}^3 r_B \frac{\rho_B(\boldsymbol{r}_B)}{|\boldsymbol{r}_A - \boldsymbol{r}_B|}, \qquad \phi_A(\boldsymbol{r}_B) = \int \mathrm{d}^3 r_A \frac{\rho_A(\boldsymbol{r}_A)}{|\boldsymbol{r}_A - \boldsymbol{r}_B|}$$
$$\rho_A(\boldsymbol{r}_A) = |\psi_A(\boldsymbol{r}_A)|^2, \qquad \rho_B(\boldsymbol{r}_B) = |\psi_B(\boldsymbol{r}_B)|^2.$$

(строчка про их идею)

Тут никак не отражено свойство тождественности электронов.

Анзац

$$\psi(\boldsymbol{r}_A, \boldsymbol{r}_B) \approx \psi_S(\boldsymbol{r}_A, \boldsymbol{r}_B) = \left\{\psi_{AB} + (-1)^S \psi_{BA}\right\}/\sqrt{2}$$

и (???? там еще обнуление одно) дает уравнения Хартри-Фока (??)

$$E_A\psi_A = \left\{-\frac{1}{2}\triangle_A - \frac{Z}{r_A} + \phi_B(\boldsymbol{r}_A)\right\}\psi_A + (-1)^S\phi(\boldsymbol{r}_A)\psi_B(\boldsymbol{r}_A),$$
$$E_B\psi_B = \left\{-\frac{1}{2}\triangle_B - \frac{Z}{r_B} + \phi_A(\boldsymbol{r}_B)\right\}\psi_B + (-1)^S\phi^*(\boldsymbol{r}_B)\psi_A(\boldsymbol{r}_B).$$

Самосогласованное поле: конфигурация электронов, термы

Основное состояние

Релятивистские поправки: электронные J-термы

Helium

(спишу у Зу потом, нужно будет - за часа 2 додумаю)

Нерелятивистская задача атома гелия

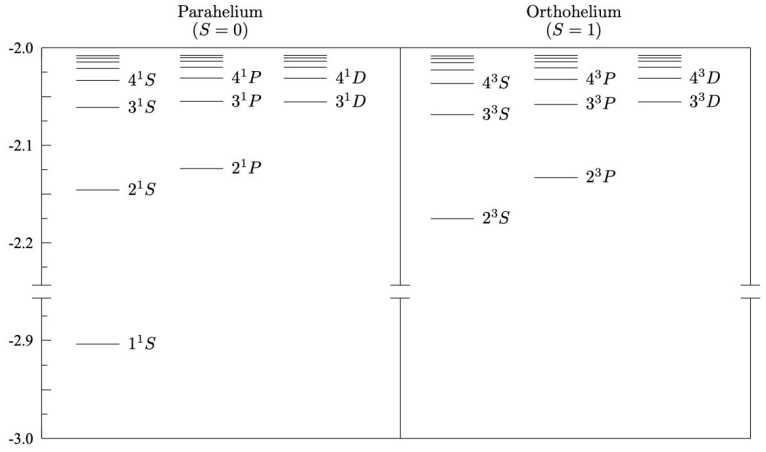
$$\hat{H}_{\mathrm{NR}} = \frac{\boldsymbol{p}_A^2}{2m} + \frac{\boldsymbol{p}_B^2}{2m} - \frac{Ze^2}{r_A} - \frac{Ze^2}{r_B} + \frac{e^2}{|\boldsymbol{r}_A - \boldsymbol{r}_B|}, \quad Z = 2,$$

$S = 0$: (para, a-sym)

$$|1,0\rangle = \frac{1}{\sqrt{2}}\left\{|+\rangle_A|-\rangle_B + |-\rangle_A|+\rangle_B\right\},$$
$$|0,0\rangle = \frac{1}{\sqrt{2}}\left\{|+\rangle_A|-\rangle_B - |-\rangle_A|+\rangle_B\right\},$$

$S = 1$: (orto, sym)

$$|1,+1\rangle = |+\rangle_A|+\rangle_B,$$
$$|1,-1\rangle = |-\rangle_A|-\rangle_B,$$



В атомных единицах (в единицах $a_{\text{Bohr}} = \hbar^2/(me^2)$, а энергия в удвоенных ридбергах $E_0 = \hbar^2/(ma^2)$, например, уровни в водороде в атомных единицах $E_n = -1/(2n^2)$).

Обменное взаимодействие

Об основных методах и уравнениях для многоэлектронного атома

Поправки к центральному потенциалу: термы

Правило интервалов Ланде. Расщепление термов вследствие спин-орбитального взаимодействия происходит с регулярными интервалами по J: разность энергий соседних термов:

$$\Delta \langle V_{ls} \rangle \equiv E\left({}^{2S+1}L_J\right) - E\left({}^{2S+1}L_{J-1}\right) = A_{LS} J \sim J. \qquad \text{(S-O interaction)}$$

(!! решу еще задачи про это!! какое обоснование этого?????)

О методе Томаса-Ферми

We consider degenerate, zero-temperature electron gas in a box of volume V, into which N electrons:

$$\frac{dN}{dk} = \frac{k^2 V}{\pi^2}$$

$$n = \frac{N}{V} = \frac{k_F^3}{3\pi^2}$$
$$k_F = \left(3\pi^2 n\right)^{1/3}.$$

$$E = \frac{\hbar^2 V k_F^5}{10 m \pi^2}$$

$$E = \frac{\hbar^2 \left(3\pi^2 N\right)^{5/3}}{10 m \pi^2} V^{-2/3}$$

$$P = \frac{\hbar^2}{15 m \pi^2} \left(3\pi^2 n\right)^{5/3}, \qquad \text{P=-d E / d V}$$

The net force per unit volume on an element of the electron fluid is the sum of $-\nabla P$ due to the pressure gradient and $\rho \mathbf{E}$ due to the electric field, where ρ is the electron charge density. These forces must balance each other in equilibrium. Since $\rho = -en$ and $\mathbf{E} = -\nabla\Phi$, where Φ is the electrostatic potential, we have the condition for hydrostatic equilibrium,

$$\nabla P = en\nabla\Phi$$

We note that the force per unit volume $-\nabla P$ will be directed outward, since the pressure must increase as we move inward, so the electrostatic force per unit volume $\rho\mathbf{E} = en\nabla\Phi$ must be directed inward. Equation (7) is augmented by the Poisson equation,

$$\nabla^2\Phi = -4\pi\rho = 4\pi ne - 4\pi Ze\delta(\mathbf{x})$$

$$\nabla P = \frac{\hbar^2}{3m}\left(3\pi^2\right)^{2/3} n^{2/3}\nabla n$$

$$\frac{\hbar^2}{3m}\left(3\pi^2\right)^{2/3} n^{-1/3}\nabla n = e\nabla\Phi$$

$$\frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3} = e\left(\Phi - \Phi_0\right) = e\Psi$$

$$\Psi = \Phi - \Phi_0$$

$$\frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3} = \frac{\hbar^2 k_F^2}{2m} = \frac{p_F^2}{2m}$$

$$\frac{p_F^2}{2m} - e\Phi = -e\Phi_0$$

(потом додумаю, см 9 страниц из университета Калифорнии, просто не до этого пока)

ротаторах (???)

(почти не решал про них)
(мб про молекулы простые тоже тут где-то будет раздел, пока не до них)

других важных свойствах атомов

О рентгеновских термах и эффекте Оже

(половину страницы добавлю, что это вообще?)

О мультипольных моментах

(см. пока ЛЛ3, пока не работал с этим, в теории сперва пропишу)

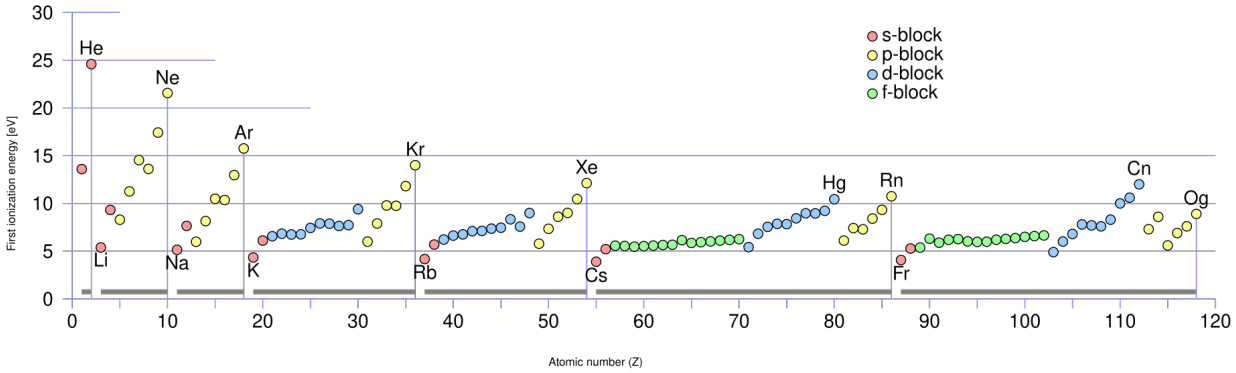
Periodic table

(просто напишу важные факты о ней для задач)

n	l	Degeneracy	N
1	0	2	2
2	0, 1	$2\times(1+3)=8$	$2+8=10$
3	0, 1, 2	$2\times(1+3+5)=18$	$2+8+18=28$
4	0, 1, 2, 3	$2\times(1+3+5+7)=32$	$2+8+18+32=60$

(см. Тонга, не уверен просто, что важные тут темы)

(см. Тонга про это, ну или много что другое)



(четкий ответ на вопрос, где нужны мультипольные моменты???)

(мб другие общие свойства из химии или таблицы менделеева добавлю)

1.4.3 Many-particle condensed systems: basics

(в статфизе и конд средах это много используется, пока там напишу, потом сюда буду переписывать)

Second quantization

$$\hat{a}_i^\dagger \left|..., n_i, ...\right\rangle = \sqrt{n_i + 1} \left|..., n_i + 1, ...\right\rangle$$
$$\hat{a}_i \left|..., n_i + 1, ...\right\rangle = \sqrt{n_i + 1} \left|..., n_i, ...\right\rangle$$

$$[\hat{a}_i, \hat{a}_j] = \hat{a}_i\hat{a}_j - \hat{a}_j\hat{a}_i = \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right] = 0, \quad \left[\hat{a}_i, \hat{a}_j^\dagger\right] = \delta_{ij} \qquad \text{for bosons,}$$
$$\{\hat{a}_i, \hat{a}_j\} = \hat{a}_i\hat{a}_j + \hat{a}_j\hat{a}_i = \left\{\hat{a}_i^\dagger, \hat{a}_j^\dagger\right\} = 0, \quad \left\{\hat{a}_i, \hat{a}_j^\dagger\right\} = \delta_{ij} \qquad \text{for fermions.}$$

Basis transformations can be readily imported from the first quantized language

$$|\lambda\rangle = \sum_i \langle i|\lambda\rangle |i\rangle \quad \Rightarrow \quad \hat{a}_\lambda^\dagger = \sum_i \langle i|\lambda\rangle \hat{a}_i^\dagger.$$

While any orthonormal basis leads to an equally valid description of a system, one basis is rather generic as many operators find a natural definition in it: the site basis $|\mathbf{r}\rangle$:

$$\langle \mathbf{r}|i\rangle = \phi_i(\mathbf{r}) \quad |\mathbf{r}\rangle : \quad \text{particle localized at } \mathbf{r}.$$

Creation and annihilation operators in this particular basis get a special name: field operators

$$\hat{\psi}^\dagger(\mathbf{r}) = \sum_i \phi_i^*(\mathbf{r}) a_i^\dagger$$

The kinetic energy:

$$\hat{T} = \sum_{ij} t_{ij} \hat{a}_i^\dagger \hat{a}_j = \sum_{ij} \hat{a}_i^\dagger \hat{a}_j \int d\mathbf{r} \phi_i^*(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} \right] \phi_j(\mathbf{r}) = \frac{\hbar^2}{2m} \int d\mathbf{r} \nabla \hat{\psi}^\dagger(\mathbf{r}) \nabla \hat{\psi}(\mathbf{r})$$

The potential energy:

$$U = \int d\mathbf{r} U(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r})$$

Two particle interactions:

$$V = \int d\mathbf{r} d\mathbf{r}' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r}')$$

And finally the Hamiltonian for particles interacting with a contact pseudo potential

$$H = \int d\mathbf{r} \left[\frac{\hbar^2}{2m} \nabla \hat{\psi}^\dagger(\mathbf{r}) \nabla \hat{\psi}(\mathbf{r}) + U(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) + \frac{4\pi a \hbar^2}{m} \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r}) \right]$$

(later I'll add more from QFT and condensed matter)

Тождественные частицы, exchange interaction

$$\psi_{ab}^{(\pm)}(\vec{r}_1, \vec{r}_2) = \psi_a(\vec{r}_1) \psi_b(\vec{r}_2) \pm \psi_a(\vec{r}_2) \Psi_b(\vec{r}_1)$$
$$E^\pm = \frac{\iint \left(\Psi_{ab}^\pm\right)^* U(x_1 x_2) \Psi_{ab}^\pm dx_1 dx_2}{\iint \left(\Psi_{ab}^\pm\right)^* \Psi_{ab}^\pm dx_1 dx_2} = A \pm J$$

(????)

Young tableaux for quantum identical particles

(Ландау писал про это, ну или Тахтаджаян, см. пока их. нужно будет - впишу, пока об этом в записи по алгебре)

Examples of properties of systems of identical particles

(про задачу с 2 или 3 электронами и их симметриями)
(очень важно, указание про задачи в духе "поместим две частицы в яму"!!)

динамике многочастичных систем

(?? как ее по итогу описывать??)

задаче двух тел и разделении переменных

(потом подумаю, куда вставить. есть приложения - тут, чисто с теор т.з. вопрос большой - смещу ниже, в указания на теорию)

Основные формулы задачи двух тел

$$H = -\frac{\hbar^2}{2m_1}\Delta_1 - \frac{\hbar^2}{2m_2}\Delta_2 + V\left(\boldsymbol{x}_1 - \boldsymbol{x}_2\right),$$

$\boldsymbol{r} := \boldsymbol{r}_1 - \boldsymbol{r}_2$, $\boldsymbol{R} := \frac{m_1}{m_1+m_2} r_1 + \frac{m_2}{m_1+m_2}\boldsymbol{r}_2$,

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta_r + V(\boldsymbol{r}) + \left\{-\frac{\hbar^2}{2\left(m_1+m_2\right)}\Delta_R + W(\boldsymbol{R})\right\}$$

$$\hat{H}_r = \frac{\hat{p}^2}{2m} + V(r), \quad \hat{\boldsymbol{p}} = -\mathrm{i}\hbar\nabla_r$$

$$\hat{H}_R = \frac{\hat{\boldsymbol{P}}^2}{2M} + W(\boldsymbol{R}), \quad \hat{\boldsymbol{P}} = -\mathrm{i}\hbar\boldsymbol{\nabla}_R,$$

$M = m_1 + m_2$.

$$\mathscr{H} = L^2\left(\mathbb{R}^6\right) \equiv L^2\left(\mathbb{R}^3, d^3\boldsymbol{X}\right) \otimes L^2\left(\mathbb{R}^3, d^3\boldsymbol{x}\right).$$

1.4.4 Addition of two angular momenta

Самосопряженный оператор $\boldsymbol{M}^2$ в гильбертовом пространстве $L^2\left(S^2, d\boldsymbol{n}\right)$ имеет чисто точечный спектр, состоящий из собственных значений $\hbar^2 l(l+1)$ кратностей $2l+1, l = 0, 1, 2, ...$, и разложение $L^2\left(S^2, d\boldsymbol{n}\right) = \bigoplus_{l=0}^{\infty} \mathscr{D}_l$ дает разложение по его собственным функциям:

$$\psi = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} C_{lm}Y_{lm}, \qquad \forall\psi \in L^2\left(S^2, d\boldsymbol{n}\right); \qquad C_{lm} := \int_0^{2\pi}\int_0^{\pi} \psi(\vartheta,\varphi)\overline{Y_{lm}(\vartheta,\varphi)}\sin\vartheta d\vartheta d\varphi$$

(еще решу про это задачу)

Основная идея и основные формулы сложения моментов

$$\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle = (-1)^{j_1 - j_2 + m}\sqrt{2j+1}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}$$

$$U(\hat{\mathbf{n}}, \theta) = e^{-i\theta\hat{\mathbf{n}}\cdot(\mathbf{J}_1+\mathbf{J}_2)/\hbar} = U_1(\hat{\mathbf{n}}, \theta)U_2(\hat{\mathbf{n}}, \theta)$$

$$U\left|j_1 j_2 m_1 m_2\right\rangle = \sum_{jm}\sum_{m'} \left|jm'\right\rangle D^j_{m'm}\left\langle jm | j_1 j_2 m_1' m_2'\right\rangle$$

$$U\left|j_1 j_2 m_1 m_2\right\rangle = U_1\left|j_1 m_1\right\rangle U_2\left|j_2 m_2\right\rangle = \sum_{m_1' m_2'}\left|j_1 j_2 m_1' m_2'\right\rangle D^{j_1}_{m_1' m_1} D^{j_2}_{m_2' m_2}$$

$$D^{j_1}_{m_1 m_1'} D^{j_2}_{m_2 m_2'} = \sum_{jmm'}\left\langle j_1 j_2 m_1 m_2 | jm\right\rangle D^j_{mm'}\left\langle jm' | j_1 j_2 m_1' m_2'\right\rangle$$

Основные свойства коэффициентов Клебша-Гордана

(пойму какие основные - напишу сюда.)

(абзац, а что если больше моментов складывается? подробно - мб во 2й 1й части.)

1.4.5 $T \neq 0$ quantum systems, black body

(см. пока статфиз)

Ensembles

Bose-Einstein distribution

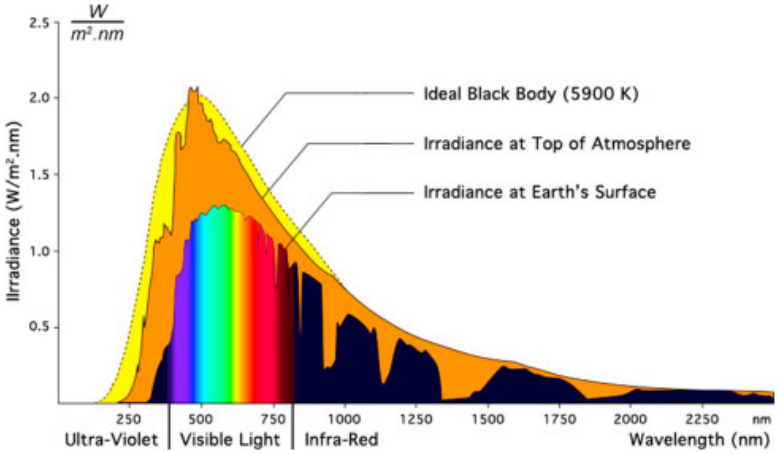
(тут всякие методы для задач, приближения, т.п.)

Fermi-Dirac distribution

(тут всякие методы для задач, приближения, т.п.)

Black body

(см статфиз пока про это, когда-то напишу и сюда. Дело 1 часа, просто не до этого)



(??? абзац, качественно почему такие пропасти в поглощении???)

Kirchhoff's law of thermal radiation:

For an arbitrary body emitting and absorbing thermal radiation in thermodynamic equilibrium, the emissivity function is equal to the absorptivity function.

or, simpler:

For a body of any arbitrary material emitting and absorbing thermal electromagnetic radiation at every wavelength in thermodynamic equilibrium, the ratio of its emissive power to its dimensionless coefficient of absorption is equal to a universal function only of radiative wavelength and temperature. That universal function describes the perfect black-body emissive power

$$\frac{B_\omega}{A_\omega} = \frac{c\rho_\omega}{4\pi}.$$

Тело, для которого $A_\omega = 1$, называется абсолютно черным; оно полностью поглощает падающее на него излучение, "перерабатывая" его в равновесное излучение с температурой, равной температуре тела. Поэтому отношение $\frac{B_\omega}{A_\omega} = \mathcal{E}_\omega$ совпадает с испускательной способностью абсолютно черного тела,

$$\mathcal{E}_\omega = \frac{c\rho_\omega}{4\pi}$$

(тут коротко напоминание формул фотометрии, потому что часто они нужны для задач излучения и определения интенсивности)

Определение, на сколько нагреется тело (?!?!)

(хз, как это сделать, но задачи про это есть, мб см. лабник.)

применении законов излучения черного тела (!!)

(есть задачи про это неочевидные, допишу про них указания)

1.5 Typical models and effects

1.5.1 Qubits, quantum computation

Осцилляции Раби

$$\hat{H} = \begin{pmatrix} E_0 + \Delta & We^{i\chi} \\ We^{-i\chi} & E_0 - \Delta \end{pmatrix}$$

$$E_\pm = E_0 \pm \sqrt{\Delta^2 + W^2}$$

$$|\psi_+\rangle = \begin{pmatrix} \cos\frac{\alpha}{2} \\ e^{-i\chi}\sin\frac{\alpha}{2} \end{pmatrix}, \quad |\psi_-\rangle = \begin{pmatrix} \sin\frac{\alpha}{2} \\ -e^{-i\chi}\cos\frac{\alpha}{2} \end{pmatrix}$$

Пусть система с гамильтонианом (1.69) при $t = 0$ находится в состоянии $|\Psi(0)\rangle = |0\rangle$, какова вероятность $P_1(t)$ обнаружить систему в состоянии $|1\rangle$ в произвольный момент времени t?

$$|\Psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = c_+ |\psi_+\rangle + c_- |\psi_-\rangle$$

$$c_+ = \langle\psi_+|\Psi(0)\rangle = \cos\frac{\alpha}{2}, \quad c_- = \langle\psi - |\Psi(0)\rangle = \sin\frac{\alpha}{2}$$

$$|\Psi(t)\rangle = \cos\frac{\alpha}{2} e^{-\frac{i}{\hbar}E_+ t} |\psi_+\rangle + \sin\frac{\alpha}{2} e^{-\frac{i}{\hbar}E_- t} |\psi_-\rangle$$

$$P_1(t) = \left| e^{-i\chi}\sin\frac{\alpha}{2} e^{-\frac{i}{\hbar}E_+ t}\cos\frac{\alpha}{2} - e^{-i\chi}\cos\frac{\alpha}{2} e^{-\frac{i}{\hbar}E_- t}\sin\frac{\alpha}{2} \right|^2 =$$

$$= \frac{\sin^2\alpha}{4} \left| e^{-\frac{i}{\hbar}E_+ t} - e^{-\frac{i}{\hbar}E_- t} \right|^2 = \sin^2\alpha \sin^2\left(\frac{E_+ - E_-}{2\hbar} t\right)$$

$\Omega := \frac{2\sqrt{\Delta^2+W^2}}{\hbar}$

$$P_1(t) = \frac{W^2}{\Delta^2 + W^2} \sin^2\left(\frac{\Omega t}{2}\right)$$

For the model

$$\hat{H} = \begin{pmatrix} E_0 + \Delta & We^{-i\omega t} \\ We^{i\omega t} & E_0 - \Delta \end{pmatrix}$$

$$P_1(t) = \frac{W^2}{(\Delta - \hbar\omega/2)^2 + W^2} \sin^2\left(\frac{\Omega t}{2}\right), \quad \Omega = \frac{2\sqrt{(\Delta - \hbar\omega/2)^2 + W^2}}{\hbar}$$

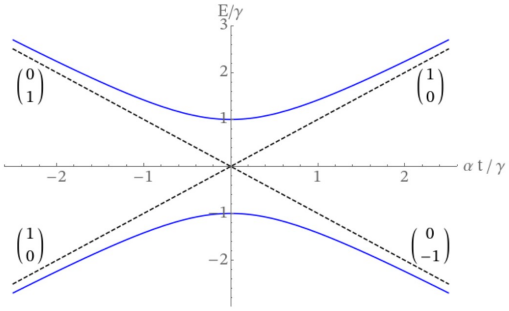
(!!! добавлю графики!!)

(см. запись по квантовой оптике с указанием на другие детали про это. также см. теор раздел, где обсужу подробно это)

Задача Ландау-Зенера

$$\hat{H} = \begin{pmatrix} \alpha t & \gamma \\ \gamma & -\alpha t \end{pmatrix}.$$

$$\psi(-\infty) \sim \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \qquad P(\psi(+\infty) = |\downarrow\rangle) = ?$$



$$\alpha \gg \gamma^2 \qquad \Rightarrow \qquad P_{1\to 2} \approx \pi \frac{\gamma^2}{\alpha}. \qquad \text{big}$$

$$\alpha \ll \gamma^2 \qquad \Rightarrow \qquad P_{1\to 2} = \#e^{-\pi\gamma^2/\alpha} \qquad \text{little}$$

Proof:

$$E_+(t) = \sqrt{\gamma^2 + (\alpha t)^2}, \quad |\psi_+(t)\rangle = \frac{1}{\sqrt{2\left(\gamma^2 + (\alpha t)^2 + \alpha t\sqrt{\gamma^2 + (\alpha t)^2}\right)}} \begin{pmatrix} \sqrt{\gamma^2 + (\alpha t)^2} + \alpha t \\ \gamma \end{pmatrix}$$

$$E_-(t) = -\sqrt{\gamma^2 + (\alpha t)^2}, \quad |\psi_-(t)\rangle = \frac{1}{\sqrt{2\left(\gamma^2 + (\alpha t)^2 - \alpha t\sqrt{\gamma^2 + (\alpha t)^2}\right)}} \begin{pmatrix} \sqrt{\gamma^2 + (\alpha t)^2} - \alpha t \\ -\gamma \end{pmatrix}$$

$$\alpha t = \gamma \sinh\theta$$

$$E_+(\theta) = \gamma\cosh\theta, \quad |\psi_+(\theta)\rangle = \frac{1}{\sqrt{2\cosh\theta}} \begin{pmatrix} e^{\theta/2} \\ e^{-\theta/2} \end{pmatrix}$$

$$E_-(\theta) = -\gamma\cosh\theta, \quad |\psi_-(\theta)\rangle = \frac{1}{\sqrt{2\cosh\theta}} \begin{pmatrix} e^{-\theta/2} \\ -e^{\theta/2} \end{pmatrix}$$

Также Ландау-Зенер имеет точное решение, получаемое методом Лапласа.
(?? решу еще раз. см. записи семинаров птф, там решена она??)
(допишу скоро)

Other features of qubits and similar bits

сфере Блоха (сфере Пуанкаре) и кубитах

(просто известный теор метод, см. кв. оптику)

Qutrits

(??? I'll write something)

Quantum computation: main methods

(see note on q inform for now)

1.5.2 De Broglie waves, photoelectric effect, Compton effect

(мб что-то еще теор про это добвлю сюда, посмотрим)

Об уравнении де Бройля и длине волны де Бройля

$$\lambda \equiv \frac{h}{p} \equiv \frac{h}{mv} \equiv \frac{h}{\sqrt{2mE}}$$

(тут про смысл ее предложения!!)

комптоновской длине волны $\lambda_c = \hbar/(mc)$

Полная энергия $E = E_K + m_0c^2$ включает кинетическую энергию E_K и энергию покоя $E_0 = m_0c^2$, в терминах которых

$$\lambda = \frac{h}{p} = hc\left[E_K\left(E_K + 2m_0c^2\right)\right]^{-1/2}$$

$$p = \frac{E}{c} = \frac{\hbar\omega}{c} = \hbar k = \frac{h}{\lambda}$$

$$p_e = \frac{mc\beta}{\sqrt{1+\beta^2}}.$$

$$T_e = \hbar\omega_0 - \hbar\omega \approx \frac{hc}{\lambda^2}\Delta\lambda$$

$$T_{\max} = T_{\text{back}} = \frac{hc}{\lambda^2}2\lambda_c = \frac{2E^2}{mc^2}$$

Частица, локализованная в области с линейными размерами не более λ_{C}, согласно соотношению неопределённостей имеет квантовомеханическую неопределённость в импульсе не менее mc и неопределённость в энергии не менее mc^2, что достаточно для рождения пар частиц-античастиц с массой m. (!?!?!? почему???)

- пи-мезона: $\bar{\lambda}_{\text{C}}^{\pi} \approx 1,46 \cdot 10^{-15}$ m (характерное расстояние ядерных взаимодействий);
- W-бозона: $\bar{\lambda}_{\text{C}}^{-\text{W}} \approx 2,45 \cdot 10^{-18}$M (характерное расстояние слабых взаимодействий).

простейших столкновениях частиц

Пишем ЗСИ и ЗСЭ, подставляем энергии электронов или фотонов.
(все для общефизных задач про них!)

Об упрощенном фотоэффекте

(формула Эйштейна)
(тут обзор моделей в пару абзацев)

фотоэффекте (!!)

Суть описания фотоэффекта

(коротко все формулы про эту задачу)

О сечении фотоэффекта (!?!?)

$$\sigma = \frac{8}{3}\pi a^2 \alpha_{\text{em}} \left(\frac{4E_{\text{at}}}{\hbar\omega_{\text{i}}}\right)^{7/2}, \qquad \left(\frac{4E_{\text{at}}}{\hbar\omega_{\text{i}}}\right)^{7/2} \ll 1,$$

Proof:

$$|\mathfrak{i}\rangle = |\boldsymbol{k}_{\text{i}}, \lambda_{\text{i}}\rangle\, |\psi_{1\ \text{s}}\rangle\,, \qquad |\mathfrak{f}\rangle = |\,\text{vac}\rangle\, |\boldsymbol{k}_{\mathfrak{f}}\rangle\,.$$

$$\langle \boldsymbol{r}|\psi_{1\ \text{s}}\rangle = \frac{1}{\sqrt{\pi a^3}} \mathrm{e}^{-r/a}.$$

$$\hat{V}(t) = -\boldsymbol{d}\cdot\hat{\mathcal{E}} = -e\boldsymbol{r}\cdot\hat{\mathcal{E}}(\boldsymbol{r},t),$$

$$\mathrm{d}w_{\text{fi}} = \frac{2\pi}{\hbar^2}\delta\left(\omega_{\text{i}} + \omega_{\text{at}} - \omega_{\text{f}}\right) |V_{\text{fi}}(0)|^2 \ \mathrm{d}\nu_{\text{f}},$$

$$\mathrm{d}\nu_{\text{f}} = \frac{\mathrm{d}^3 k_{\text{f}}}{(2\pi)^3},$$

$$\hbar\omega_{\text{f}} = \frac{\hbar^2 k_f^2}{2m},$$

$$\hbar\omega_{\text{at}} = -\frac{\hbar^2}{2ma^2}$$

$$\hat{\mathcal{E}}(\boldsymbol{r}, t=0) = \int \frac{\mathrm{d}^3 k_{\mathbb{E}}}{(2\pi)^3} \frac{\mathrm{i}}{2} \left\{ \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \boldsymbol{\epsilon}_\lambda(\boldsymbol{k}) \mathfrak{a}_\lambda(\boldsymbol{k}) - \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \boldsymbol{\epsilon}^*_\lambda(\boldsymbol{k}) \mathfrak{a}^\dagger_\lambda(\boldsymbol{k}) \right\}$$

$$V_{\text{fi}}(0) = -\mathrm{i}e \frac{\partial}{\partial \boldsymbol{k}_{\text{f}}} \int \mathrm{d}^3 r \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_{\text{f}}\cdot\boldsymbol{r}} \frac{1}{\sqrt{\pi a^3}} \mathrm{e}^{-r/a} \mathrm{i}\hbar\omega_{\text{i}} \boldsymbol{\epsilon}_{\lambda_{\text{i}}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}_{\text{i}}\cdot\boldsymbol{r}}$$

$$(qa)^2 \approx (k_{\text{f}} a)^2 \gg 1,$$

$$V_{\text{fi}}(0) \approx -2^5 \pi \hbar\omega_{\text{i}} \frac{e}{\sqrt{\pi a^3}} \left(\boldsymbol{\epsilon}_{\lambda_{\text{i}}} \cdot \boldsymbol{k}_{\mathfrak{f}}\right) \frac{a^5}{(k_{\text{f}} a)^6},$$

$$\Pi^{\alpha\beta} = \sum_{\lambda_{\text{i}}} \epsilon^\alpha_{\lambda_{\text{i}}} \left(\epsilon^\beta_{\lambda_{\text{i}}}\right)^* = \delta^{\alpha\beta} - k_{\text{i}}^\alpha k_{\text{i}}^\beta / \boldsymbol{k}_{\text{i}}^2. \qquad \left(\left(k_{\text{i}}\right)_\alpha \Pi^{\alpha\beta} = 0, \right)$$

$$\frac{1}{2}\sum_{\lambda_{\text{i}}} |V_{\mathfrak{f}\mathfrak{i}}(0)|^2 = 2^7 \pi^2 \frac{\hbar^4}{m^2} \frac{e^2}{\pi a^3} \frac{a^6}{\left(k_{\mathfrak{f}} a\right)^8} k_{\mathfrak{f}}^2 \left(1 - \frac{\left(\boldsymbol{k}_{\mathfrak{f}} \cdot \boldsymbol{k}_{\text{i}}\right)^2}{k_{\mathfrak{f}}^2 k_{\text{i}}^2}\right).$$

$$w_{\text{fi}} = \int_0^{2\pi} \mathrm{d}\phi \int_{-1}^{1} \mathrm{d}\cos\theta \cdot \left(1 - \cos^2\theta\right) \int_0^\infty \frac{k_{\text{f}}^2\, \mathrm{d}k_{\text{f}}}{(2\pi)^3} \frac{2\pi}{\hbar^2} \delta\left(\omega_{\text{i}} - \frac{\hbar k_{\text{f}}^2}{2m}\right) 2^9 \pi^2 \frac{\hbar^5 c}{m^2} \alpha_{\text{em}} \frac{a}{\left(k_{\text{f}} a\right)^6} =$$

$$= 2\pi \cdot \frac{4}{3} \cdot \frac{k_{\text{f}}^2}{(2\pi)^3} \frac{2\pi}{\hbar^2} \frac{m}{\hbar k_{\text{f}}} 2^9 \pi^2 \frac{\hbar^5 c}{m^2} \alpha_{\text{em}} \frac{a}{\left(k_{\text{f}} a\right)^6} =$$

$$= \frac{2^{10}}{3} \pi \frac{\hbar^2 c}{m} \alpha_{\text{em}} \frac{1}{\left(k_{\text{f}} a\right)^5}.$$

Полное сечение фотоэффекта σ выражается через вероятность квантового перехода в единицу времени и поток фотонов

$$j_\mathrm{i} = c \cdot 2\hbar\omega_\mathrm{i},$$

так что

$$\sigma = \frac{w_\mathrm{fi}}{j_\mathrm{i}}.$$

В рассматриваемой задаче

$$j_\mathrm{i} = c \cdot \frac{\hbar^2 k_\mathrm{f}^2}{m},$$

и

$$\sigma = \frac{2^{10}}{3}\pi a^2 \alpha_\mathrm{em} \frac{1}{(k_\mathrm{f} a)^7} = \pi a^2 \alpha_\mathrm{em} \frac{2^{10}}{3} \frac{1}{(k_\mathrm{f} a)^7}.$$

$$\sigma = \frac{8}{3}\pi a^2 \alpha_\mathrm{em} \left(\frac{4E_\mathrm{at}}{\hbar\omega_\mathrm{i}}\right)^{7/2} \qquad \frac{2^7}{(k_\mathrm{f} a)^7} = \left(\frac{4E_\mathrm{at}}{\hbar\omega_\mathrm{i}}\right)^{7/2} \ll 1,$$

(абзац про другие свойства, а также про экспериментальные результаты. пока не актуально, потом додумаю.)

О влиянии фотоэффекта на разные процессы и применениях

(отсылка ко многим задачам Овчинкина, да и вообще многие эксперименты по нему ставятся)

О других фотоэффектах

(мб допишу, пока не до этого, мб есть они, там внутренний, т.п.)

Об эффекте Комптона (!!!)

(очень годно нужно прописать)

О типичном эффекте Комптона

$$\lambda_\text{расс.} - \lambda_\text{пад.} = \Lambda_\mathrm{K}(1 - \cos\theta),$$
$$\Lambda_\mathrm{K} := \frac{h}{mc} = 2,42 \cdot 10^{-10}\text{см}.$$

Он получается из ЗСЭ и ЗСИ:

$$mc^2 + \hbar\omega_0 = \gamma mc^2 + \hbar\omega_1,$$
$$\frac{\hbar\omega_0}{c} = \gamma mv\cos\varphi + \frac{\hbar\omega_1}{c}\cos\theta$$
$$\gamma mv \sin\varphi = \frac{\hbar\omega_1}{c}\sin\theta$$

Тут считаем, что электрон покоится вначале и проецируем импульсы на две оси - так что имеем два уравнения. (???? еще раз это сделаю.)

Об обратном эффекте Комптона

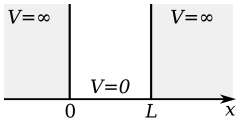
(встетилось, укажу)

О другом про эффект Комптона

1.5.3 1D scatterings and bound states

моделях связных состояний

1D wall with infinite walls



$$\psi'' + \frac{2m}{h^2}(E - U(x))\psi(x) = 0 \qquad \psi(0) = \psi(a) = 0$$

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin \frac{\pi n}{a} x, & x \in \{0, a\} \\ 0, & x \notin \{0, a\} \end{cases},$$

$$k: \quad ka = \pi n, \quad n \in \mathbb{N},$$

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2ma^2}.$$

$$\langle x \rangle = \int_0^a dx \psi^2(x) x = \frac{a}{2}, \qquad \rho(x) = 1/a$$

$$\langle x^2 \rangle = \int_0^a dx \psi^2(x) x^2 = \frac{a^2}{3} - \frac{a^2}{2\pi^2 n^2}$$

$$(\Delta x)^2 = \frac{a^2}{12}\left(1 - \frac{6}{\pi^2 n^2}\right), \qquad \overline{(\Delta \hat{x})^2} = \frac{a^2}{12}$$

$$(\Delta p)^2 = \langle p^2 \rangle = \langle 2mE_n \rangle = \frac{\hbar^2}{a^2}\pi^2 n^2.$$

То есть имеем просто равномерное распределение, но с квантовыми поправками, которые свои для каждого энергетического уровня.

$$(\Delta x)^2 (\Delta p)^2 = \frac{\hbar^2}{12}\left(\pi^2 n^2 - 6\right) \geqslant \frac{\hbar^2}{4},$$

$$\Delta\Gamma|_{\Delta n = 1} = \frac{d\Delta\Gamma}{dn}\Delta n \to \frac{\hbar}{2\sqrt{3}}\pi.$$

В импульсном представлении:

$$\psi_n(p) \equiv \langle p|n\rangle = \int_0^1 \langle p|x\rangle\langle x|n\rangle dx = \int_0^1 \frac{1}{\sqrt{2\pi}} e^{-ipx}\sqrt{2}\sin n\pi x dx = -i2\sqrt{\pi}\mathrm{e}^{-i\frac{(p-n\pi)}{2}} \frac{n\sin\left(\frac{p-n\pi}{2}\right)}{p^2 - (n\pi)^2}.$$

В квазиклассическом приближении ($n \gg 1$) вблизи $p = \pm n\pi$

$$|\psi_n(p)|^2 \simeq \frac{\sin^2(\varepsilon/2)}{\pi\varepsilon^2}, \qquad \int_{-\infty}^{\infty} \frac{\sin^2(\varepsilon/2)}{\pi\varepsilon^2} d\varepsilon = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} dx = \frac{1}{2},$$

$\varepsilon = p \pm n\pi$, что соответствует классической плотности вероятности распределения по импульсам:

$$\rho(p) = \frac{1}{2}\delta\left(p - p_n\right) + \frac{1}{2}\delta\left(p + p_n\right), \quad p_n = \sqrt{2E_n} = \pi n.$$

О типичных одномерных ямах

(по идее тут заготовка к задачам овчинкина)

В симметричной потенциальной яме $V_1 = V_2 = V$ при любых V и a всегда имеется по крайней мере один уровень. (решал про это задачу)

(тут про особенности мелкой ямы!)

О средних значениях (?!?!)

(для тривиальных задач указания)

В трехмерном пространстве при описании системы волновой функцией $\langle A \rangle = \int\limits_V |\psi|^2 A dV$, $dV = 4\pi r^2 dr$.

(?? слышал, что средние могут становиться бесконечностью, что тогда? не знаю. проверить нужно, действительно ли в тогда волновая функция в $L^2(U)$, U - область определения системы. мб всегда и окажется, что нет, она не в этой области? не знаю в общем, наверняка с этим могут быть проблемы)

О мелкой яме (!?!??!!?)

(!! словами допишу указание про потенциал)

$$U_0 \ll \hbar^2/ma^2$$

$$\frac{p^2}{2m}\psi(p) + U_p \int (dp')\,\psi(p') \approx E\psi(p)$$

$$\psi(\boldsymbol{p}) = -\frac{U_{\boldsymbol{p}}}{-E + \frac{p^2}{2m}} \int (d\boldsymbol{p}')\,\psi(\boldsymbol{p}') = -\frac{U_{\boldsymbol{p}}}{-E + \frac{p^2}{2m}},$$

$$|U_{p=0}| \int \frac{(dp)}{|E| + \frac{p^2}{2m}} \approx 1$$

$|U_{\boldsymbol{p}=0}| = -U_{\boldsymbol{p}=0}, \quad |E| = -E.$

При $d = 1$ всегда есть уровень: имеем $|U_{\boldsymbol{p}=0}| \sqrt{\frac{m}{2|E|}} = 1$, получаем

$$|E| = \frac{m}{2\hbar^2} \left| \int\limits_{-\infty}^{\infty} U(x) dx \right|^2$$

При $d = 2$ уровень мелкий, из $\int \frac{d^2p}{(2\pi)^2} \frac{1}{|E| + \frac{p^2}{2m}} = \int \frac{2\pi p dp}{4\pi^2} \frac{1}{|E| + \frac{p^2}{2m}} \approx \frac{m}{\pi} \int\limits_{\sim\sqrt{mE}}^{\sim 1/a} \frac{dp}{p} = \frac{m}{2\pi} \ln \frac{\#}{ma^2|E|}$ (???? масштаб обрезания введен???? что с расходимостью???) получаем

$$|E| = \#\frac{\hbar^2}{ma^2} \exp\left(-\frac{2\pi\hbar^2}{m} \left| \int U(r) d^2 r \right|^{-1} \right)$$

(???? непонятно откуда минус и $\hbar$ мы почему-то восстанавливаем?? что делать с $\#$?? в общем, задача точно не дорешена.)

При $d \geq 3$ связных состояний нет. Доказательство: на больших импульсах $\int \frac{(dp)}{|E| + \frac{p^2}{2m}}$ может быть обрезан на $\sim 1/a$; Имеем $\int \frac{(dp)}{|E| + \frac{p^2}{2m}} \sim ma^{2-d}$ и $U_{p=0} \sim U_0 a^d$; поэтому $\int \frac{(dp)}{|E| + \frac{p^2}{2m}} U_{p=0} \sim \frac{U_0}{\hbar^2/ma^2} \ll 1$. Сделать это выражение порядка единицы, изменяя энергию, невозможно, вот и видим, что уравнение самосогласования не имеет решений. (??????? оценку интеграла пока что не понял???? подумаю лучше про это потом.)

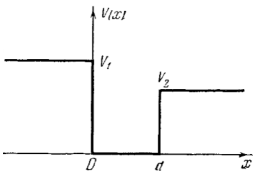
Об элементарных моделях рассеяния (!!!!)

(тут к общефизу заготовки!!!)

Рассеяние на ступеньке:

Рассеяние на яме

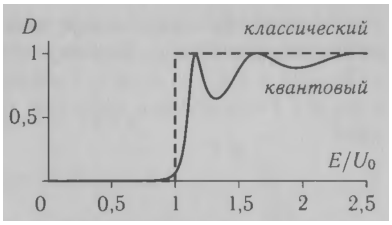
Для потенциала



(!! скоро впишу ответ!)

Надбарьерные и подбарьерные отражения (!!)

$$U(x) = \begin{cases} -U_0, & |x| < a/2 \\ 0, & |x| > a/2 \end{cases}$$



D в квантовом случае достигает $D = 1$ (классический предел) лишь при $k_1 a = \pi n,\ n = 1, 2, ...$

Proof:

$$\psi(x) = \begin{cases} e^{ikx} + Ae^{-ikx}, & x < -a/2, \\ Ce^{ik_1 x} + De^{-ik_1 x}, & |x| < a/2, \\ Be^{ikx}, & x > a/2, \end{cases} \qquad \begin{aligned} k^2 &:= \frac{2mE}{\hbar^2} > 0, \\ k_1^2 &:= \frac{2m\left(E + U_0\right)}{\hbar^2}. \end{aligned}$$

$\psi_{x=\pm a/2+0} = \psi_{x=\pm a/2-0}, \quad \psi'_{x=\pm a/2+0} = \psi'_{x=\pm a/2-0} \quad \Rightarrow$

$$A = \frac{ie^{-ika}\left(k_1^2 - k^2\right)\sin k_1 a}{2kk_1 \cos k_1 a - i\left(k_1^2 + k^2\right)\sin k_1 a}, \qquad B = \frac{2kk_1 e^{-ik_1 a}}{2kk_1 \cos k_1 a - i\left(k_1^2 + k^2\right)\sin k_1 a}.$$

$$R = \frac{\left|j_x^{\text{ref}}\right|}{\left|j_x^{\text{in}}\right|} = |A|^2 = \frac{\left(k_1^2 - k^2\right)\sin^2 k_1 a}{4k_1^2 k^2 \cos^2 k_1 a + \left(k_1^2 + k^2\right)^2 \sin^2 k_1 a} = \frac{\left(k_1^2 - k^2\right)\sin^2 k_1 a}{4k_1^2 k^2 + \left(k_1^2 - k^2\right)^2 \sin^2 k_1 a}.$$

$$D = \frac{\left|j_x^{\text{tr}}\right|}{\left|j_x^{\text{in}}\right|} = |B|^2 = \frac{4k_1^2 k^2}{4k_1^2 k^2 \cos^2 k_1 a + \left(k_1^2 + k^2\right)^2 \sin^2 k_1 a} = \frac{4k_1^2 k^2}{4k_1^2 k^2 + \left(k_1^2 - k^2\right)^2 \sin^2 k_1 a}.$$

$D + R = 1.$

$$U(x) = \begin{cases} 0, & |x| > a/2, \\ U_0, & |x| < a/2, \end{cases}$$

we take the solutions above and set $k_1^2 = \frac{2m}{\hbar^2}(E + U_0)$ осуществить замену $U_0 \to -U_0$. При $0 < E < U_0$ нужно дополнительно положить $k_1 = i\varkappa_1$, $\varkappa_1^2 = \frac{2m}{\hbar^2}(U_0 - E)$. В результате получаем

$$R = \frac{(\varkappa^2 + k^2)\,\mathrm{sh}^2\,\varkappa_1 a}{4\varkappa_1^2 k^2 + (\varkappa_1^2 + k^2)^2\,\mathrm{sh}^2\,\varkappa_1 a}, \qquad D = \frac{4\varkappa_1^2 k^2}{4\varkappa_1^2 k^2 + (\varkappa_1^2 + k^2)^2\,\mathrm{sh}^2\,\varkappa_1 a}$$

Models with δ-potentials

δ-potential

(впишу скоро, см. пока задачи)
Bound states:

$$\psi_0(p) \equiv \langle p|0\rangle = \int\limits_{-\infty}^{\infty} dx \langle p|x\rangle\langle x|0\rangle = \frac{\sqrt{\varkappa_0}}{(2\pi\hbar)^{1/2}} \int\limits_{-\infty}^{\infty} e^{-\varkappa_0|x| - \frac{ipx}{\hbar}} dx = \sqrt{\frac{2}{\pi}} \frac{(\varkappa_0\hbar)^{3/2}}{(\varkappa_0\hbar)^2 + p^2}$$

$$\psi(x) = \sqrt{\varkappa}\exp(-\varkappa|x|)$$

Scattering:

$$t = \frac{1}{1 - \frac{m\lambda}{i\hbar^2 k}}, \qquad r = \frac{1}{\frac{i\hbar^2 k}{m\lambda} - 1}.$$

$$R = |r|^2 = \frac{1}{1 + \frac{\hbar^4 k^2}{m^2\lambda^2}}, \qquad T = |t|^2 = 1 - R = \frac{1}{1 + \frac{m^2\lambda^2}{\hbar^4 k^2}}$$

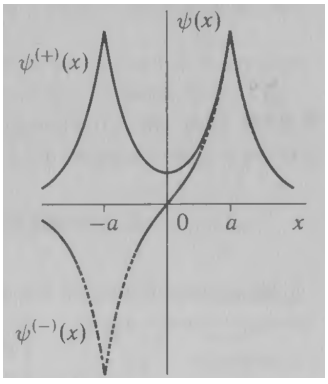
$$U(x) = -\frac{\hbar^2}{m} x_0 \delta(x)$$

Переобозначим $x^2 = \frac{2m|E|}{\hbar^2}$

$$\psi''(x) - \left(x^2 - 2x_0\delta(x)\right)\psi(x) = 0$$

$\psi(+0) = \psi(-0)$
$\psi'(+0) - \psi'(-0) = -2x_0\psi(0)$
$j(+0) = j(-0)$

Double δ-potential



$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x) \qquad V(x)=-q\left[\delta\left(x+\frac{R}{2}\right)+\lambda\delta\left(x-\frac{R}{2}\right)\right]$$

wavefunction matching,

$$\psi(x)=Ae^{-d|x+\frac{R}{2}|}+Be^{-d|x-\frac{R}{2}|}. \quad R=2$$

$$\begin{vmatrix} q-d & qe^{-dR} \\ q\lambda e^{-dR} & q\lambda-d \end{vmatrix}=0, \qquad \text{where } E=-\frac{d^2}{2}.$$

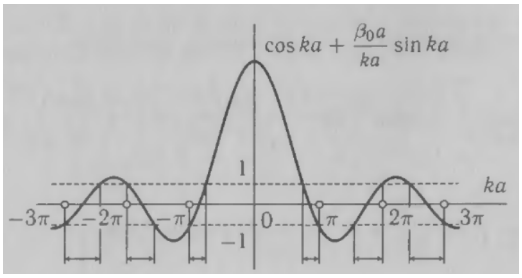
$$d_\pm(\lambda)=\frac{1}{2}q(\lambda+1)\pm\frac{1}{2}\left\{q^2(1+\lambda)^2-4\lambda q^2\left[1-e^{-2d_\pm(\lambda)R}\right]\right\}^{1/2}$$

$$d_\pm=q\left[1\pm e^{-d_\pm R}\right].$$

Moving δ-potential

Kroning-Penny model $U(x)=\sum\limits_{n=-\infty}^{\infty}\frac{\hbar^2\beta_0}{m}\delta(x-na)$

(??)



1.5.4 Oscillator

Основные формулы

$$H=-\frac{\hbar^2}{2m}\frac{d^2}{dq^2}+\frac{m\omega^2q^2}{2}=\hbar\omega\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)$$

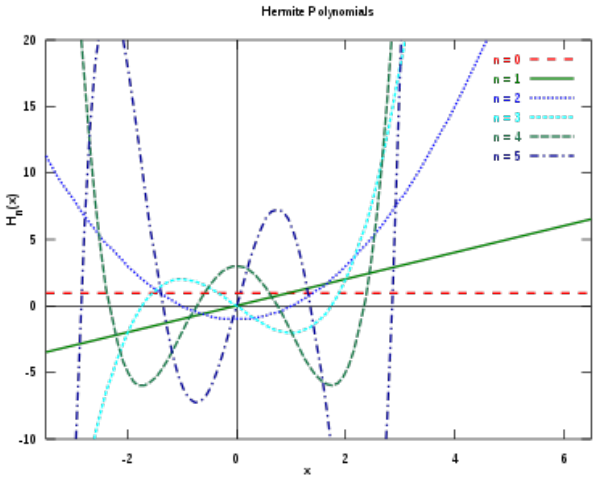
$$a=\frac{1}{\sqrt{2\omega\hbar}}(\omega Q+iP), \qquad a^*=\frac{1}{\sqrt{2\omega\hbar}}(\omega Q-iP)$$

$$\hat{x}=\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}+\hat{a}^\dagger\right) \qquad \hat{p}=-i\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a}-\hat{a}^\dagger\right)$$

$$[a,a^*]=I$$

$$\psi_0(x) = \frac{1}{(\pi\ell^2)^{1/4}} e^{-\xi^2/2}, \qquad h_1(x) = \frac{2\xi}{(4\pi\ell^2)^{1/4}} e^{-\xi^2/2},$$
$$\psi_2(x) = \frac{2\xi^2 - 1}{(4\pi\ell^2)^{1/4}} e^{-\xi^2/2}, \qquad h_3(x) = \frac{2\xi^3 - 3\xi}{(9\pi\ell^2)^{1/4}} e^{-\xi^2/2}$$

$\omega = \sqrt{\frac{k}{m}}, \qquad \ell = \sqrt{\frac{\hbar}{m\omega}}, \qquad \xi = \frac{x}{\ell}$



$$\psi_n(q) = \sqrt[4]{\frac{m\omega}{\pi\hbar}} \frac{1}{\sqrt{2^n n!}} e^{-\frac{m\omega}{2\hbar}q^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}} q\right) =$$
$$= \frac{(a^*)^n}{\sqrt{n!}} \psi_0 \equiv \frac{1}{\sqrt{n!}} \left(\frac{1}{\sqrt{2\omega\hbar}} \left(\omega q - \hbar \frac{d}{dq}\right)\right)^n \psi_0$$

Proof: $y = x\sqrt{\frac{m\omega}{\hbar}}$ и $E = \hbar\omega\left(\epsilon + \frac{1}{2}\right)$, получаем $\psi''(y) + (2\epsilon + 1 - y^2)\,\psi(y) = 0$, потом заменой $y = \sqrt{z}$,

$$4z\psi''(z) + 2\psi'(z) + (2\epsilon + 1 - z)\psi(z) = 0.$$
$$\psi(z) = \chi(z)e^{-z/2}$$
$$z\chi''(z) + \left(\frac{1}{2} - z\right)\chi'(z) + \frac{\epsilon}{2}\chi(z) = 0$$
$$\chi(z) = C_1 \cdot {}_1F_1\left(-\frac{\epsilon}{2}; \frac{1}{2}; z\right) + C_2\sqrt{z} \cdot {}_1F_1\left(-\frac{\epsilon - 1}{2}; \frac{3}{2}; z\right) \qquad b = \frac{1}{2}, a = -\frac{\epsilon}{2}$$

В общем случае ${}_1F_1 \sim e^z$, что соответствует экспоненциально растущей волновой функции и нас не устраивает, поэтому ряд должен обрываться.

(!!! подробнее про этот обрыв ряда!!!)

Осцилляторная теорема - Волновая функция n-того возбуждённого состояния содержит ровно n узлов (нулей волновой функции). Так, например, основное состояние узлов вовсе не содержит.

(??????????????)

Для a, a^* и $N = a^*a$

$$[N, a] = -a, \quad [N, a^*] = a^*, \quad [a, a^*] = I$$

(???????)

Это неприводимое унитарное представление четырехмерной разрешимой алгебры Ли $\tilde{\mathfrak{h}}$, ассоциированной с алгеброй Гейзенберга $\mathfrak{h} = \mathfrak{h}_1$: $\tilde{\mathfrak{h}}$ - алгебра Ли с образующими e, f, h, и c, e, f, c удовлетворяют соотношениям алгебры Гейзенберга $\mathfrak{h}$ и

$$[h, e] = -f, \quad [h, f] = \omega^2 e, \quad [h, c] = 0.$$

(?????)

Неприводимое интегрируемое представление ρ алгебры Гейзенберга $\mathfrak{h}$ (?????) продолжается до унитарного представления алгебры Ли $\tilde{\mathfrak{h}}$, если положить $\rho(h) = -i\omega N = \frac{P^2+\omega^2 Q^2}{2i\hbar} + \frac{i\omega}{2} I$.

В инвариантных терминах алгебра Ли $\tilde{\mathfrak{h}}$ - одномерное правое расширение алгебры Гейзенберга $\mathfrak{h}$,

$$0 \to \mathfrak{h} \to \tilde{\mathfrak{h}} \to \mathbb{R} \to 0.$$

Оно определяется $\mathfrak{h}$-значным 1-коциклом $r \in Z^1(\mathfrak{h}, \mathfrak{h})$ на алгебре Ли - дифференциальным оператором на $\mathfrak{h}$, задаваемым на образующих формулой

$$r(e) = f, \quad r(f) = -\omega^2 e, \quad r(c) = 0.$$

Конкретно, если $h \in \tilde{\mathfrak{h}}$ таково, что $\bar{h} = 1 \in \mathbb{R}$ при проекции $\tilde{\mathfrak{h}} \to \mathbb{R}$, то, отождествляя элементы $\mathfrak{h}$ с их образами при вложении $\mathfrak{h} \hookrightarrow \tilde{\mathfrak{h}}$, имеем

$$[x + \alpha h, y + \beta h] = [x, y] - \alpha r(y) + \beta r(y), \quad x, y \in \mathfrak{h}.$$

(!! из ЛШ выпишу важные формулы, уже решил задачу ту!!!)

Solution осциллятора в сферических координатах

(тут очень нетривиальные методы, потом пропишу их, пока это в задаче написано)

Об осцилляторе с n степенями свободы

$$H = -\frac{\hbar^2}{2m}\Delta + \sum_{j=1}^{n} \frac{m\omega_j^2 q_j^2}{2}$$

$$E_{n_x n_y n_z} = \frac{2n_x + 2n_y + 2n_z + 3}{2}\hbar\omega$$

$$\psi_{n_x n_y n_z} = h_{n_x}(x) h_{n_y}(y) h_{n_z}(z)$$

$$\lambda_k = \hbar\omega_1 \left(k_1 + \frac{1}{2}\right) + ... + \hbar\omega_n \left(k_n + \frac{1}{2}\right)$$

моделях с осциллятором

Часто есть какое-то возмущение зависящее от x, тогда просто расписываем его через операторы рождения, уничтожения и по теории возмущений находим поправки. Нужно только аккуратно преобразовывать их.

(!! кстати, добавлю пару заготовок преобразований сюда!)

Quantum Quench of a Harmonic Oscillator by Tong:

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}\omega_0^2 x^2 = \hbar\omega_0\left(a_0^\dagger a_0 + \frac{1}{2}\right)$$

$a_0 = \frac{1}{\sqrt{2m\omega_0}}(m\omega_0 x + ip)$

$$\tau \ll \hbar/\omega_0 \qquad H = \frac{p^2}{2m} + \frac{1}{2}\omega^2 x^2 = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$$

$$|\emptyset\rangle = \sum_{n=0}^{\infty} \alpha_{2n}|2n\rangle \qquad \alpha_{2n+2} = \sqrt{\frac{2n+1}{2n+2}}\left(\frac{\omega-\omega_0}{\omega+\omega_0}\right)\alpha_{2n}$$

We can also address more detailed questions about the dynamics. Suppose that the quench takes place at time $t = 0$. Working in the Heisenberg picture, we know that

$$\langle\emptyset|x^2(0)|\emptyset\rangle = \frac{\hbar}{2m\omega_0} \qquad \langle\emptyset|p^2(0)|\emptyset\rangle = \frac{\hbar m\omega_0}{2}$$

$$x(t) = x(0)\cos(\omega t) + \frac{p(0)}{m\omega}\sin(\omega t)$$

$$\langle\emptyset|x\left(t_2\right)x\left(t_1\right)|\emptyset\rangle = \frac{\hbar}{2m\omega}\left[e^{-i\omega(t_2-t_1)} + \frac{\left(\omega^2-\omega_0^2\right)\cos\left(\omega\left(t_2+t_1\right)\right) + \left(\omega-\omega_0\right)^2\cos\left(\omega\left(t_2-t_1\right)\right)}{2\omega\omega_0}\right]$$

The quench term not T-invariant. The state carries a memory of the traumatic event that happened during the quench.

(????)

применениях осциллятора

(абзац про квантовые поля, типа это основная модель для них)

(короткий абзац, что если действует сила, то решаем через какую-то функцию, забыл....)

Coherent states (????)

$$T(a) := e^{-ia\hat{p}}, \qquad S(b) := e^{ib\hat{x}}$$

$$(T(a)\psi)(x) = \psi(x-a), \quad (T(a)\phi)(p) = e^{-iap}\phi(p)$$
$$(S(b)\psi)(x) = e^{ibx}\psi(x), \quad (S(b)\phi)(p) = \phi(p-b)$$

$$S(b)T(a) = e^{iab}T(a)S(b)$$

$$W(a,b) := e^{i(b\hat{x}-a\hat{p})}$$

$$W(a,b) = e^{iab/2}T(a)S(b) = e^{-iab/2}S(b)T(a)$$

$$|a,b\rangle := W(a,b)|0\rangle$$

$$W(x,p) = \exp(i(p\hat{x} - x\hat{p})) = \exp\left(za^\dagger - \bar{z}a\right) \equiv D(z)$$

$$D(z) = e^{-|z|^2/2} \exp\left(za^\dagger\right) \exp(-\bar{z}a)$$

$$|z\rangle = e^{-|z|^2/2} \exp\left(za^\dagger\right)|0\rangle = e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}}|n\rangle.$$

$$\langle z|\hat{n}|z\rangle = \langle z|a^\dagger a|z\rangle = z^* z\langle z|z\rangle = |z|^2$$
$$\langle z|\hat{n}^2|z\rangle = \langle z|a^\dagger a a^\dagger a|z\rangle = |z|^2\langle z|aa^\dagger|z\rangle = |z|^4 + |z|^2$$
$$U(t)|z\rangle = e^{-it/2}\left|e^{-it}z\right\rangle$$

$$\langle w|z\rangle = e^{w^* z} e^{-|z|^2/2} e^{-|w|^2/2}$$

$$|\langle w|z\rangle|^2 = e^{-|w-z|^2}$$

$$\int \frac{dxdp}{2\pi}|z\rangle\langle z| = 1 \qquad \text{overcomplete}$$

$$\frac{1}{2\pi}\int dxdp e^{-|z|^2} \frac{z^n (z^*)^m}{\sqrt{n!m!}} = \int d|z|^2 e^{-|z|^2} \int \frac{d\varphi}{2\pi} \frac{z^n (z^*)^m}{\sqrt{n!m!}}$$

Coherent states are ubiquitous in nature, because they are generically produced by classically driving a harmonic oscillator:

$$x(t) = x_0(t) + \int dt' \sin(t-t')\,\theta(t-t')\,f(t')$$

$$\hat{x}(t) = \frac{\hat{a}e^{-it} + \hat{a}^\dagger e^{it}}{\sqrt{2}} + \int dt' \frac{i\theta(t-t')\,f(t')}{2}\left(e^{-i(t-t')} - e^{-i(t-t')}\right)$$

$$\hat{x}(t) = \frac{1}{\sqrt{2}}\left(\left(\hat{a} + \frac{i}{\sqrt{2}}\tilde{f}(1)\right)e^{-it} + \left(\hat{a}^\dagger - \frac{i}{\sqrt{2}}\tilde{f}(-1)\right)e^{it}\right)$$

(??!! конкретно, где они используются! примеры с формулами)

голоморфном представлении (?????)

(пока не нужно никогда было, и не усвоено еще.)

фермионном осцилляторе

Суть (??)

применения фермионного осциллятора (??)

(зачем он нужен????)

другом про осциллятор

О важности осциллятора для понимания квантования

(часто эта модель используется, так что пару абзацев напишу, как же так?)

1.5.5 Motion in a central field, hydrogen

Основное об атоме водорода

Основные формулы центрального поля и водорода

A.e. длины (боровский радиус): $a = \frac{\hbar^2}{m_e e^2} = 0,529 \cdot 10^{-8}$c.
A.e. энергии: $E_a = \frac{e^2}{a} = \frac{m_e e^4}{\hbar^2} = 27,21$ эВ.
A. e. скорости: $v_a = \frac{e^2}{\hbar} = 2,2 \cdot 10^8$ cm/c.
A. e. времени: $\tau_a = \frac{\hbar a}{e^2} = \frac{\hbar^3}{m_e e^4} = 2,42 \cdot 10^{-17}$c.
A. e. частоты: $\nu_a = \frac{m_e e^4}{\hbar^3} = 4,13 \cdot 10^{16}$c^{-1}.
A. e. напряженности электрического поля: $\varepsilon_a = \frac{e}{a^2} = 5,14 \cdot 10^9$ В/ см.

$$E_n = -\mathrm{Rg} \cdot \frac{Z^2}{n^2},$$

$\mathrm{Rg} := 2\pi\hbar c R = \frac{me^4}{2\hbar^2} = \frac{e^2}{2a_0} = 13,60$ эВ $= 2,179 \cdot 10^{-18}$ Дж,

$$E_{j,n} \approx -\frac{\mu c^2 \alpha^2}{2n^2}\left[1 + \frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)\right] \qquad \text{Sommerfeld fine-str. f}$$

$$R_{10} = 2\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-Zr/a_0},$$

$$R_{21} = \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_0}\right)^{\frac{3}{2}}\left(\frac{Zr}{a_0}\right) e^{-Zr/2a_0}, \quad R_{20} = 2\left(\frac{Z}{2a_0}\right)^{\frac{3}{2}}\left(1 - \frac{Zr}{2a_0}\right) e^{-Zr/2a_0}$$

$$\psi_{2,1,0} = \frac{1}{4\sqrt{2\pi}a_0^{3/2}}\frac{r}{a_0}\mathrm{e}^{-r/2a_0}\cos\theta$$

$$\psi_{2,1,\pm1} = \mp\frac{1}{8\sqrt{\pi}a_0^{3/2}}\frac{r}{a_0}\mathrm{e}^{-r/2a_0}\sin\theta e^{\pm i\varphi}$$

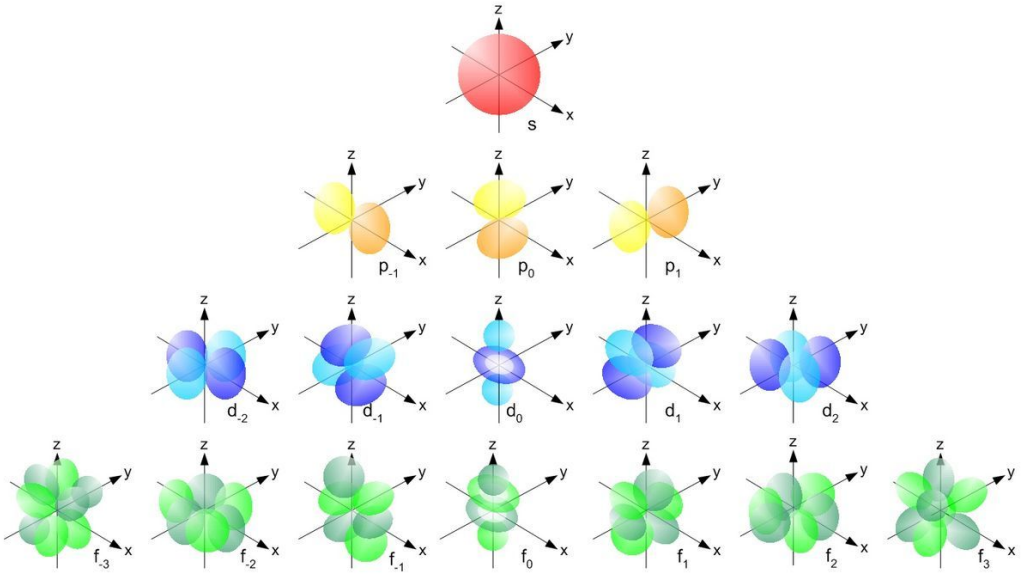
(???)

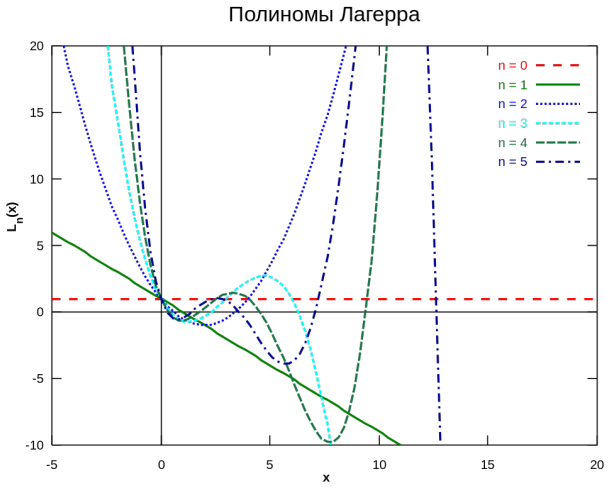
$$\mathrm{Degeneracy} = 2_{\mathrm{spin}}\sum_{l=0}^{n-1} 2l+1 = 2n^2$$

$$\psi_{n\ell m}(r,\theta,\varphi) = \sqrt{\left(\frac{2}{na_0^*}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}}\mathrm{e}^{-\rho/2}\rho^\ell L_{n-\ell-1}^{2\ell+1}(\rho)Y_\ell^m(\theta,\varphi)$$

where:
- $\rho = \frac{2r}{na_0^*}$,
- a_0^* is the reduced Bohr radius, $a_0^* = \frac{4\pi\varepsilon_0\hbar^2}{\mu e^2}$,
- $L_{n-\ell-1}^{2\ell+1}(\rho)$ is a generalized Laguerre polynomial of degree $n-\ell-1$, and

- $Y_\ell^m(\theta,\varphi)$ is a spherical harmonic function of degree ℓ and order m.





(абзац словами напишу свойства)
(!!!!!!!!!!!!! абзац про вырожденность уровней!!! сразу этот вопрос и возникает!)
Считаем водород так: $\Delta\psi + \frac{2m}{\hbar^2}[E - U(r)]\psi = 0$,(??? формула для лапласиана??),

$$\frac{\hbar^2}{2m}\left[-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{\widehat{\mathbf{l}}^2}{r^2}\psi\right] + U(r)\psi = E\psi,$$

$\widehat{\mathbf{l}}^2 = -\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\varphi}\right)\right].$

$$\widehat{p}_r\psi := -i\hbar\frac{1}{r}\frac{\partial}{\partial r}(r\psi) = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\psi$$

$$\widehat{H} = \frac{1}{2m}\left(\widehat{p}_r^2 + \frac{\hbar^2\widehat{\mathbf{l}}^2}{r^2}\right) + U(r),$$

$$\psi = R(r)Y_{lm}(\theta,\varphi)$$

$\widehat{\mathbf{1}}^2 Y_{lm} = l(l+1)Y_{lm}$,

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{l(l+1)}{r^2}R + \frac{2m}{\hbar^2}[E - U(r)]R = 0$$

$$R(r) = \frac{\chi(r)}{r}$$

$$\frac{d^2\chi}{dr^2} + \left[\frac{2m}{\hbar^2}(E-U) - \frac{l(l+1)}{r^2}\right]\chi = 0$$

$$U_l(r) = U(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2},$$

$$R_l \approx \text{ const } \cdot r^l.$$

$$\begin{aligned}\left\langle r^{-1}\right\rangle &= 0,\\ \langle r\rangle &= \frac{a}{2}\left[3n^2 - l(l+1)\right].\\ \left\langle r^2\right\rangle &= \frac{a^2n^2}{2}\left[5n^2 + 1 - 3l(l+1)\right].\end{aligned}$$

$$\frac{s+1}{n^2}\left\langle r^s\right\rangle - a(2s+1)\left\langle r^{s-1}\right\rangle + \frac{s}{4}a^2\left\{(2l+1)^2 - s^2\right\}\left\langle r^{s-2}\right\rangle = 0 \qquad s > -2l-1 \text{ (Cramers)}$$

(??? idea of the proof???)

$\frac{\partial E_n}{\partial l} = \left\langle \frac{\partial \hat{H}}{\partial l}\right\rangle_n \quad \Rightarrow \quad -\frac{\hbar^2}{2ma^2}\frac{\partial}{\partial l}\frac{1}{(n_r+l+1)^2} = \left\langle \frac{\hbar^2}{2m}\frac{\partial}{\partial l}\frac{l(l+1)}{r^2}\right\rangle \quad \Rightarrow \quad \left\langle \frac{1}{r^2}\right\rangle = \frac{2}{a^2}\frac{1}{n^3(2l+1)}$.

Из интегрирования уравнения Шредингера (?? мб добавлю формулу, по см. Киселева):

$$|\Psi(0)|^2 = \frac{m}{2\pi\hbar^2}\langle V'\rangle.$$

(??? Тут я хз про средние, оно странно вычисляется, нужно тренироваться дальше в этом.)

При учёте движения ядра масса электрона заменяется приведённой массой электрона и ядра и тогда $R_i = \frac{R_\infty}{\frac{1+m}{M_i}}$, M_i - масса ядра атома.

разложении плоских волн

$$\begin{aligned}e^{\mathrm{i}kr\cos\theta} &= \sum_l (2l+1)P_l(\cos\theta)(-\mathrm{i})^l\frac{r^l}{2\mathrm{i}k^{l+1}}\left(\frac{1}{r}\frac{d}{dr}\right)^l\frac{1}{r}\left\{-e^{-\mathrm{i}kr} + e^{\mathrm{i}kr}\right\} \simeq\\ &\overset{r\to\infty}{\simeq} \sum_l (2l+1)P_l(\cos\theta)\frac{1}{2\mathrm{i}kr}\left\{e^{\mathrm{i}kr} - (-1)^l e^{-\mathrm{i}kr}\right\} =\\ &= \sum_l (2l+1)P_l(\cos\theta)\ \mathrm{i}^l\ \frac{\sin\left(kr - \frac{\pi}{2}l\right)}{kr}\end{aligned}$$

$$e^{i\mathbf{kr}} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l} i^l j_l(kr)Y^*_{lm}\left(\frac{\mathbf{k}}{k}\right)Y_{lm}\left(\frac{\mathbf{r}}{r}\right)$$

$$\sigma_l = \frac{\pi}{k^2}(2l+1).$$

При больших значениях l сумма прицельных площадей по интервалу Δl значений l (такому, что $1 \ll \Delta l \ll l$) равна

$$\sum_{\Delta l} \sigma_l \approx \frac{\pi}{k^2} \cdot 2l\Delta l = 2\pi \frac{l\hbar^2}{p^2}\Delta l.$$

разложении сферических волн

(тут суть пар 33 ЛЛ3)

$$\frac{1}{r}\frac{d^2(rR_{kl})}{dr^2} + k^2 R_{kl} = 0.$$

$$R_{kl} \approx 2\frac{\sin(kr - l\pi/2 + \delta_l)}{r},$$

$$R_{kl} = (-1)^l \cdot 2\frac{r^l}{k^l}\left(\frac{d}{rdr}\right)^l \frac{\sin kr}{r}$$

$$R_{kl} \equiv \sqrt{\frac{2\pi k}{r}} J_{l+1/2}(kr) = 2kj_l(kr); \qquad j_l(x) := \sqrt{\frac{\pi}{2x}} J_{l+1/2}(x)$$

$$j_0 = \frac{\sin x}{x}, \qquad j_1 = \frac{\sin x}{x^2} - \frac{\cos x}{x}, \qquad j_2 = \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin x - \frac{3\cos x}{x^2}.$$

$$R^{\pm}_{kl} = (-1)^l A \frac{r^l}{k^l}\left(\frac{1}{r}\frac{d}{dr}\right)^l \frac{e^{\pm ikr}}{r} = \pm iA\sqrt{\frac{k\pi}{2r}} H^{(1,2)}_{l+1/2}(kr) \approx \frac{A}{r}\exp\left[\pm i\left(kr - \frac{\pi l}{2}\right)\right].$$

$$R^{\pm}_{kl} \approx A\frac{(2l-1)!!}{k^l} r^{-l-1}. \qquad (r \to 0)$$

Движение в центральном поле по Ландау

(см. его пар 35, там всякие спецфункции, нетривиальные методы! потом подумаю - пропишу в теорию и сюда.)

Другие общие свойства атома водорода

Водород в электрическом поле (ЛЛ.77)

$$E = -\frac{1}{2n^2} + \frac{3}{2}\mathcal{E}n(n_1 - n_2) - \frac{\mathcal{E}^2}{16}n^4\left[17n^2 - 3(n_1 - n_2)^2 - 9m^2 + 19\right]$$

(?? как понимать формулу?)

Proof:

$$\left(\frac{1}{2}\Delta + E + \frac{1}{r} - \mathcal{E}z\right)\psi = 0.$$

parabolic:
$$\frac{d}{d\xi}\left(\xi\frac{df_1}{d\xi}\right)+\left(\frac{E}{2}\xi-\frac{m^2}{4\xi}-\frac{\mathcal{E}}{4}\xi^2\right)f_1-\beta_1 f_1$$
$$\frac{d}{d\eta}\left(\eta\frac{df_2}{d\eta}\right)+\left(\frac{E}{2}\eta-\frac{m^2}{4\eta}+\frac{\mathcal{E}}{4}\eta^2\right)f_2-\beta_2 f_2,\quad \beta_1+\beta_2=1$$

(дальше словами напишу, в ЛЛ3 вывод на страницы 4)

Например, вероятность ионизации водорода считается так:
(см. задачу ЛЛ3 пар 77, пока не думал про неё особо, чуть что разберусь!)

Скрытая $SO(4)$ симметрия (??)

$$H:=\frac{\boldsymbol{P}^2}{2}-\frac{\alpha}{r},$$
$$\hat{\boldsymbol{W}}:=\frac{1}{2}(\boldsymbol{P}\times\boldsymbol{M}-\boldsymbol{M}\times\boldsymbol{P})-\frac{\alpha\boldsymbol{Q}}{r}$$ вектор Лапласа-Рунге-Ленца
$$W_j=\frac{1}{2}\varepsilon_{jkl}\left(P_kM_l+M_lP_k\right)-\frac{\alpha Q_j}{r},\quad j=1,2,3.$$

Здесь Q_i - операторы умножения на x_i, и все время подразумевается суммирование по повторяющимся индексам $1,2,3$. В силу коммутационных соотношений (3.5) имеем также

$$\boldsymbol{W}=\boldsymbol{P}\times\boldsymbol{M}-\frac{\alpha\boldsymbol{Q}}{r}-i\hbar\boldsymbol{P}=-\boldsymbol{M}\times\boldsymbol{P}-\frac{\alpha\boldsymbol{Q}}{r}+i\hbar\boldsymbol{P},$$

где слагаемое $i\hbar\boldsymbol{P}$ играет роль «квантовой поправки». Следующий результат выявляет скрытую симметрию кулоновской задачи.

Предложение 5.1. Оператор Шрёдингера H атома водорода имеет шесть квантовых интегралов движения $\boldsymbol{M}$ и $\boldsymbol{W}$,

$$[H,M_i]=[H,W_i]=0,\quad i=1,2,3,$$

удовлетворяющих условиям $\boldsymbol{W}\cdot\boldsymbol{M}=\boldsymbol{M}\cdot\boldsymbol{W}=0$ и $\boldsymbol{W}^2=\alpha^2+2H\boldsymbol{M}^2+2\hbar^2H$.

Кроме того, самосопряженные операторы $\boldsymbol{M}$ и $\boldsymbol{W}$ удовлетворяют

$$[M_j,M_k]=i\hbar\varepsilon_{jkl}M_l,\quad [W_j,M_k]=i\hbar\varepsilon_{jkl}W_l,\quad [W_j,W_k]=-2i\hbar\varepsilon_{jkl}M_lH$$

Хорошо известно из теории представлений группы Ли SO(4), что сферические гармоники - это ограничения на S^3 однородных гармонических многочленов на $\mathbb{R}^4$ степени $n-1, n\in\mathbb{N}$. Соответственно, уравнение (5.26) получается как предел $|\boldsymbol{u}|\to 1$ формулы Грина для однородных гармонических функций степени $n-1$ в единичном шаре в $\mathbb{R}^4$ с использованием потенциала двойного слоя. Это дает $\lambda=n$, чем опять устанавливается точная формула для уровней энергии атома водорода. Изоморфизм $\mathscr{H}_0\simeq L^2\left(S^3,d\Omega\right)$ следует из (5.27), а (5.23) - из разложения

$$L^2\left(S^3,d\Omega\right)\simeq\bigoplus_{l\in\frac{1}{2}\mathbb{Z}\geqslant 0}V_l\otimes V_l$$

регулярного представления SO(4) в прямую сумму неприводимых компонент. Можно также получить явный вид (5.4) собственных функций, воспользовавшись теорией представлений SO(4).

1.5.6 Fine structure, Zeeman, Stark effects

Overview of perturbations for hydrogen

The perturbations to the hydrogen energy levels, are of order:

$$\text{fine structure: } \alpha^2, \qquad \text{Lamb: } \alpha^3 \log\frac{1}{\alpha}, \qquad \text{Zeeman: } \alpha B, \qquad \text{hyperfine: } \alpha^2\frac{m_e}{m_p}$$

$$\alpha \sim 10^{-2}, \qquad m_e/m_p \sim 10^{-3},$$

(?? check this!) and the fine structure is suppressed by $O(10)$ numeric factors. The hydrogen energy levels themselves are $\sim \alpha^2 mc^2$.

In positronium there are modifications: the fine structure is still α^2, but the Lamb shift enters at the same order, since there is a tree-level diagram where the electron and positron annihilate and reappear; the Lamb shift for hydrogen is loop-level. The hyperfine splitting also enters at order α^2, so one must account for all of these effects at once.

(тут обзор, что со Штарком и Зееманом в итоге)

Поправки от тонкой структуры в случае общего центрального поля:

$$\delta V = -\frac{\boldsymbol{p}^4}{8m^3c^2} + \frac{e^2\hbar}{2m^2c^2}\frac{1}{r^3}(\boldsymbol{s}\cdot\boldsymbol{L}) + \frac{e^2\hbar^2}{2m^2c^2}\pi\delta(\boldsymbol{r}).$$

Тут первый член - кинетический, из разложения $E^2 = p^2c^2 + m^2c^4$ по c. Второй - (? от магнитного взаимодействия???) Последний член - контактный, от (???), а в случае неточечности ядра вместо дельта-функции имеем распределение заряда в ядре конечного радиуса (? решу эту модель еще раз).

Их получаем из $\hat{H} = \frac{p^2}{2m} + e\Phi - \frac{p^4}{8m^3c^2} + \frac{e\hbar}{2m^2c^2}\frac{\Phi'(r)}{r}(\boldsymbol{s}\cdot\boldsymbol{L}) + \frac{e\hbar^2}{8m^2c^2}\Delta\Phi$, где для атома водорода подставляем $\Phi = -\frac{e}{r}$, $\Phi'(r) = \frac{e}{r^2}$, и $\triangle\Phi(r) = 4\pi e\delta(\boldsymbol{r})$.

Fine structure:

$$(\Delta E)_{n,j} = \frac{(Z\alpha)^4 mc^2}{2}\left(\frac{3}{4n} - \frac{2}{2j+1}\right)\frac{1}{n^3}$$

(!!!!!!!!!!!!! тут обзор, что если такое-то есть поле, то такие-то члены в гамильтониане!!!)

Derivation of the part of corrections (?)

Relativistic Motion

$$E = \sqrt{\mathbf{p}^2c^2 + m^2c^4} \approx mc^2 + \frac{\mathbf{p}^2}{2m} - \frac{\mathbf{p}^4}{8m^3c^2} + \ldots$$

$$\Delta H = -\frac{\mathbf{p}^4}{8m^3c^2}$$

$$\langle nlm|\Delta H\,|nl'm'\rangle = 0 \quad \text{unless } l = l' \text{ and } m = m'$$

$$(\Delta E_1)_{n,l} = \langle\Delta H\rangle_{n,l}$$

$\langle \Delta H \rangle_{n,l} = \langle nlm|\Delta H|nlm\rangle$

$$\Delta H = -\frac{1}{2mc^2}[H - V(r)]^2$$

$$(\Delta E_1)_{n,l} = -\frac{1}{2mc^2}\left[E_n^2 - 2E_n\langle V(r)\rangle_{n,l} + \left\langle V(r)^2\right\rangle_{n,l}\right]$$

$\langle E\rangle = \langle T\rangle + \langle V\rangle = \frac{1}{2}\langle V\rangle$.

$$\left\langle \frac{1}{r}\right\rangle_{n,l} = -\frac{1}{Z\alpha\hbar c}\langle V\rangle_{n,l} = -\frac{1}{Z\alpha\hbar c}2E_n = \frac{Z}{a_0}\frac{1}{n^2}$$

$$\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + \frac{\lambda}{r^2} = \frac{\hbar^2}{2m}\frac{l'(l'+1)}{r^2}$$

$$E(l') = -mc^2(Z\alpha)^2\frac{1}{2(k+l'+1)^2}$$

$n = k + l + 1$

$$E(l') = E_n + (Z\alpha)^2 mc^2\left[\frac{1}{(k+l'+1)^3}\frac{dl'}{d\lambda}\right]\Big|_{\lambda=0}\lambda + ...$$

$$= E_n + \frac{Z^2}{a_0^2}\frac{2\lambda}{n^3(2l+1)} + ...$$

$$\left\langle \frac{1}{r^2}\right\rangle_{n,l} = \frac{Z^2}{a_0^2}\frac{2}{n^3(2l+1)}$$

$$(\Delta E_1)_{n,l} = -\frac{(Z\alpha)^4 mc^2}{2}\left(\frac{n}{l+1/2} - \frac{3}{4}\right)\frac{1}{n^4}$$

Spin-Orbit Coupling and Thomas Precession

$$\mathbf{m} = -g\frac{e}{2m}\mathbf{S}$$

$$E = -\mathbf{B}\cdot\mathbf{m}$$

$$\mathbf{B} = \frac{\gamma}{c^2}\mathbf{v}\times\mathbf{E}$$

$$\Delta E = -\frac{e\gamma}{mc^2}(\mathbf{v}\times\nabla\phi)\cdot\mathbf{S} = -\frac{e}{(mc)^2}\frac{\partial\phi}{\partial r}(\mathbf{p}\times\hat{\mathbf{r}})\cdot\mathbf{S} = \frac{e}{(mc)^2}\frac{1}{r}\frac{\partial\phi}{\partial r}\mathbf{L}\cdot\mathbf{S}$$

$\mathbf{ep} = m\gamma\mathbf{v}$

$$\Delta H_{SO} = \frac{e}{(mc)^2}\frac{1}{r}\frac{\partial\phi}{\partial r}\mathbf{L}\cdot\mathbf{S}$$

(про прецессию Томаса - указание в теории поля, тут только финальные формулы пишу, ну и в паре слов смысл явления)

$$\frac{\partial\mathbf{S}}{\partial t} = \boldsymbol{\omega}_T\times\mathbf{S} \quad \text{with} \quad \boldsymbol{\omega}_{\mathrm{T}} = \frac{\mathbf{v}\times\mathbf{a}}{2\mathrm{c}^2}$$

$$\omega_T = \frac{\gamma^2}{\gamma+1}\frac{\mathbf{v}\times\mathbf{a}}{2c^2}$$

Connection of Thomas Precession and the Spin-Orbit Coupling

$$\frac{\partial \mathbf{S}}{\partial t} = \mathbf{B}\times\mathbf{S}$$

$$\frac{\partial \mathbf{S}}{\partial t} = \mathbf{B}\times\mathbf{S} + \boldsymbol{\omega}_T\times\mathbf{S}$$

$$E = \frac{e}{m}\mathbf{B}\cdot\mathbf{S} + \boldsymbol{\omega}_T\cdot\mathbf{S}$$

$$\boldsymbol{\omega}_T\cdot\mathbf{S} = \frac{e}{2mc^2}(\mathbf{v}\times\nabla\phi)\cdot\mathbf{S} = -\frac{e}{2(mc)^2}\frac{1}{r}\frac{\partial\phi}{\partial r}\mathbf{L}\cdot\mathbf{S}$$

$$\Delta H_{SO} = \frac{e}{2(mc)^2}\frac{1}{r}\frac{\partial\phi}{\partial r}\mathbf{L}\cdot\mathbf{S}$$

Computing the Spin-Orbit Energy Shift:

$$\begin{aligned}\mathbf{L}\cdot\mathbf{S}\,|n,j,m_j;l\rangle &= \frac{\hbar^2}{2}\left(j(j+1)-l(l+1)-\frac{3}{4}\right)|n,j,m_j;l\rangle \\ &= \frac{\hbar^2}{2}\begin{cases} -(l+1)\,|n,j,m_j;l\rangle & j=l-\frac{1}{2} \\ l\,|n,j,m_j;l\rangle & j=l+\frac{1}{2}\end{cases} \qquad (l\neq 0)\end{aligned}$$

$$(\Delta E_2)_{n,j;l} = \langle \Delta H_{SO}\rangle_{n,j;l}$$

$\langle \Delta H_{SO}\rangle_{n,j;l} = \langle n,j,m_j;l|\,\Delta H_{SO}\,|n,j,m_j;l\rangle$.

$$(\Delta E_2)_{n,j;l} = -\frac{Ze^2\hbar^2}{4.4\pi\epsilon_0(mc)^2}\begin{Bmatrix} -(l+1) \\ l\end{Bmatrix}\left\langle\frac{1}{r^3}\right\rangle_{n,j;l}$$

$$\tilde{p} = -i\hbar\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)$$

$$\begin{aligned}H &= -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\right)+\frac{\hbar^2 l(l+1)}{2mr^2}-\frac{Ze^2}{4\pi\epsilon_0 r} \\ &= \frac{\tilde{p}^2}{2m}+\frac{\hbar^2 l(l+1)}{2mr^2}-\frac{Ze^2}{4\pi\epsilon_0 r}\end{aligned}$$

$$[\tilde{p},H] = -i\hbar\left(-\frac{\hbar^2 l(l+1)}{mr^3}+\frac{Ze^2}{4\pi\epsilon_0 r^2}\right)$$

$$\left\langle\frac{1}{r^3}\right\rangle_{n,j;l} = \frac{Z}{a_0}\frac{1}{l(l+1)}\left\langle\frac{1}{r^2}\right\rangle_{n,j;l} = \left(\frac{Z}{a_0}\right)^3\frac{1}{l\left(l+\frac{1}{2}\right)(l+1)}\frac{1}{n^3} \quad (l\neq 0)$$

$$(\Delta E_2)_{n,j;l} = \frac{(Z\alpha)^4 mc^2}{4}\begin{Bmatrix} -\frac{1}{j+1} \\ \frac{1}{j}\end{Bmatrix}\frac{1}{j+\frac{1}{2}}\frac{1}{n^3}$$

$$(\Delta E_1)_{n,l} = -\frac{(Z\alpha)^4 mc^2}{2}\left(\begin{Bmatrix} \frac{1}{j+1} \\ \frac{1}{j}\end{Bmatrix}-\frac{3}{4n}\right)\frac{1}{n^3}$$

$$(\Delta E_1)_{n,l} + (\Delta E_2)_{n,j;l} = \frac{(Z\alpha)^4 mc^2}{2}\left(\frac{3}{4n} - \frac{2}{2j+1}\right)\frac{1}{n^3}$$

Считаем возмущения так:

$$\hat{\mathbf{L}}\cdot\hat{\mathbf{S}} = \frac{1}{2}\left(\hat{\mathbf{J}}^2 - \hat{\mathbf{L}}^2 - \hat{\mathbf{S}}^2\right)$$

$$\langle ls;j,m|\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}|ls;j,m\rangle = \frac{\hbar^2}{2}(j(j+1) - l(l+1) - s(s+1)) =$$
$$\overset{s=1/2}{=} \frac{\hbar^2}{2}\left(j(j+1) - l(l+1) - \frac{3}{4}\right) \qquad j = l \pm 1/2$$

Zitterbewegung and the Darwin Term

$$V(\mathbf{r}) = V(\mathbf{r}_0) + \langle\Delta\mathbf{r}\rangle\cdot\frac{\partial V}{\partial\mathbf{r}} + \frac{1}{2}\langle\Delta r_i\Delta r_j\rangle\frac{\partial^2 V}{\partial r_i\partial r_j} + \ldots$$

$$\langle\Delta r_i\Delta r_j\rangle = \left(\frac{\lambda}{2}\right)^2\delta_{ij}$$

$$\Delta H_{\text{Darwin}} = \frac{\hbar^2}{8m^2c^2}\nabla^2 V \overset{1/r}{\to} \frac{Z\alpha\hbar^3}{8m^2c}4\pi\delta^3(\mathbf{r})$$

$$(\Delta E_3)_{n,l} = \langle\Delta H_{\text{Darwin}}\rangle_{n,l} = \frac{Z\alpha\hbar^3\pi}{2m^2c}\left|\psi_{nlm}(r=0)\right|^2$$

$$R_{n,l=0}(r) = -\sqrt{\left(\frac{2Z}{na_0}\right)^3\frac{(n-1)!}{2n(n!)^3}}e^{-r/na_0}L_n^1(2r/na_0)$$

$L_n^1(x) = dL_n(x)/dx$
$L_n(x) \approx n! - n!nx + \mathcal{O}(x^2)$ so that $L_n^1(0) = n!n$.

$$|\psi_{n,l=0}(0)|^2 = \frac{Z^3}{a_0^3\pi n^3}$$

$$(\Delta E_3)_{n,l} = \frac{(Z\alpha)^4 mc^2}{2}\frac{1}{n^3}\delta_{l0}$$

Derivation of fine structure from Dirac's equation together from Kiselev

Main idea:

$$E_{n,j} = mc^2\left(1 + \left(\frac{Z\alpha}{n - j - \frac{1}{2} + \sqrt{\left(j+\frac{1}{2}\right)^2 - (Z\alpha)^2}}\right)^2\right)^{-1/2}$$
$$E_{n,j} = mc^2\left(1 - (Z\alpha)^2\frac{1}{2n^2} + (Z\alpha)^4\left(\frac{3}{4n} - \frac{2}{2j+1}\right)\frac{1}{2n^3} + \ldots\right)$$

Key steps in derivation:
(спишу скоро у него, особая теория, интересная, но Тонга хватает для понимания)

Lamb shift for hydrogen atom

Consider an atom in a large cubical box of side length L:

$$\underbrace{|\mathbf{E}_k|^2 L^3}_{\text{rand class field}} \sim \underbrace{\hbar\omega_k}_{\text{vac energ}}$$

characteristic time of change: $\tau \sim 1/\omega_k$,

displsm of a particle $$\delta r \sim \frac{e\,|\mathbf{E}_k|\,\tau^2}{m} \sim \frac{e\,|\mathbf{E}_k|}{m\omega_k^2}$$

$$\langle \delta r^2 \rangle \sim \sum_{\mathbf{k}} \frac{e^2\,|\mathbf{E}_k|^2}{m^2\omega_k^4} \sim \frac{e^2\hbar}{m^2} \sum_{\mathbf{k}} \frac{1}{(L\omega_k)^3} \sim \frac{e^2\hbar}{m^2} \int d\mathbf{k} \left(\frac{L}{\hbar}\right)^3 \frac{1}{(L\omega_k)^3} \sim \frac{e^2}{m^2\hbar^2c^3} \int \frac{d\mathbf{k}}{k^3}$$

We get rid of logarithm divergence, by putting cutoffs. Modes with wavelengths larger than the atom don't affect the electron much, just pushing on it adiabatically, while modes with wavelengths smaller than the electron's Compton wavelength will instead cause new particles to spontaneously pop out of the vacuum. The ratio between these two scales is α (????), so

$$\langle \delta r^2 \rangle \sim \frac{e^2}{m^2\hbar^2c^3} \log\frac{1}{\alpha}$$

$$\frac{\Delta E}{E_n} \sim \alpha^3 \log\frac{1}{\alpha}$$

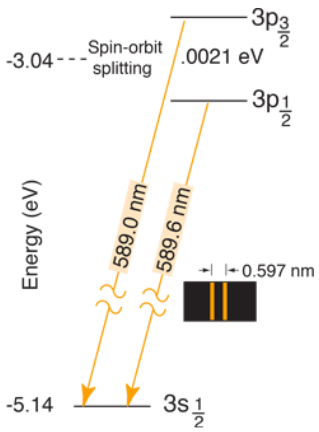
Following the same reasoning as for the Darwin term (???), this gives an energy shift of

$$\frac{\Delta E}{E_n} \sim \alpha^3 \log\frac{1}{\alpha} \qquad \text{for } \ell = 0 \text{ states.}$$

One should keep in mind that "quantum fluctuations" don't generally behave like classical stochastic ones, so in some other effects this approach does not work (????).

Об эффекте Зеемана (!!!!!)

Overview of Zeeman effects



The normal Zeeman effect is observed in systems with closed shells of electrons and arises due to lifting of the orbital degeneracy by an external magnetic field of moderate strength.

$$W_H = -\mu_H H = g m_J \mu_\mathrm{B} H,$$

уровень, отвечающий заданному J, расщепляется на $2J+1$ подуровней. Смещение уровней в единицах $\mu_\mathrm{B} H$ определяется величиной $g m_J$.

Например, жёлтый дублет натрия - переходы из $3^2P_{1/2}$ в $3^2S_{1/2}$-состояние (линия D_1), и из $3^2P_{3/2}$ - в то же $3^2S_{1/2}$-состояние (линия D_2).

Терм	L	S	J	g	m_J	gm_J
$3^2S_{1/2}$	0	1/2	1/2	2	$1/2; -1/2$	$1; -1$
$3^2P_{1/2}$	1	1/2	1/2	2/3	$1/2; -1/2$	$1/3; -1/3$
$3^2P_{3/2}$	1	1/2	3/2	4/3	$3/2; 1/2; -1/2; -3/2$	$2; 2/3; -2/3; -2$

Тут есть примеры, чуть что, в них и буду разбираться (очень подродбная теория там): https://physicspages.com/TOC%20-%20Quantum%20mechanics.html

Normal Zeeman effect (aka strong-field, aka Paschen–Back effect, aka $L+2S$ Zeeman) (!?!?!!??)

$$H = H_0^\mathrm{at} + \sum_f \left\{ \mu_0 \boldsymbol{\mathcal{H}} \cdot (\boldsymbol{l}_f + 2\boldsymbol{s}_f) + \frac{e^2}{8mc^2} \left(\boldsymbol{\mathcal{H}} \times \boldsymbol{r}_f\right)^2 \right\},$$

$$V_\mathrm{mag} = \mu_0 \mathcal{H} \cdot (\boldsymbol{L} + 2\boldsymbol{S}),$$

$$V_\mathrm{d} = \frac{e^2}{8mc^2} \sum_f \left(\boldsymbol{\mathcal{H}} \times \boldsymbol{r}_f\right)^2 = \frac{e^2 \mathcal{H}^2}{8mc^2} \sum_f r_f^2 \sin^2\theta_f$$

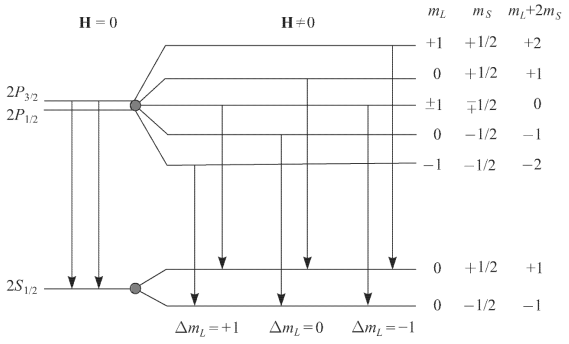
$$\widehat{H} = \widehat{H}_0 + \frac{|e|}{2mc} \mathbf{H} \sum_a [\mathbf{r}_a \widehat{\mathbf{p}}_a] + \frac{e^2}{8mc^2} \sum_a [\mathbf{H}\mathbf{r}_a]^2 + \frac{|e|\hbar}{mc} \mathbf{H}\widehat{\mathbf{S}}.$$

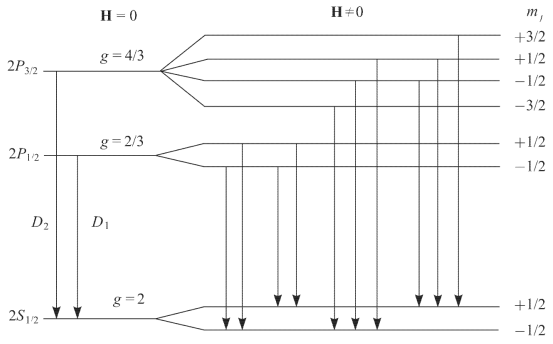
$$\widehat{H} = \widehat{H}_0 + \mu_B (\mathbf{L} + 2\widehat{\mathbf{S}})\mathbf{H} + \frac{e^2}{8mc^2} \sum_a [\mathbf{H}\mathbf{r}_a]^2$$

$$\widehat{\mu}_\mathrm{at} = -\mu_B (\widehat{\mathbf{L}} + 2\widehat{\mathbf{S}})$$

If $S = 0$, $g = 1$ (because $J = L$) and so the magnetic moment is independent of L and the upper and lower levels are split by the same amount. In this case we observe the normal Zeeman effect.

Below left - normal. right - anomalous Zeeman effects:





However, when $S \neq 0$, the value of g depends on both L and S, and so the upper and lower levels in the spectroscopic transition are split by different amounts. This is illustrated in Fig. 3.7. Note that the allowed transitions are further restricted by the angular momentum conservation selection rules, $\Delta M_J = 0$ (corresponding to emission of linearly polarized light) or $\Delta M_J = \pm 1$ (corresponding to circularly polarized light).

If the applied field is very strong, the coupling between S and L can be broken in favor of their direct coupling to the magnetic field. S and L then precess independently about the field direction. The electromagnetic field which induces the electronic transition couples only to the orbital distribution of the electrons, and so the presence of the spin does not show up in the transitions. Therefore the spectrum switches back from the anomalous to the normal Zeeman effect. This change in the spectrum is known as the Paschen-Back effect.

$$\boldsymbol{m} = -g\mu_{\mathrm{B}} M_J.$$

$$g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

$$\langle \mathbf{L} + 2\mathbf{S} \rangle = \left\langle \left(1 + \frac{\mathbf{S}\cdot\mathbf{J}}{J^2}\right)\mathbf{J} \right\rangle = \left[1 + \frac{j(j+1) - \ell(\ell+1) + s(s+1)}{2j(j+1)}\right]\langle \mathbf{J} \rangle.$$

- For one-electron atoms, some of the $2s$ states are also degenerate with the $2p$ states, as $|\ell m_\ell m_s\rangle = \left|00\tfrac{1}{2}\right\rangle$ is degenerate with $\left|10\tfrac{1}{2}\right\rangle$, and $\left|00,-\tfrac{1}{2}\right\rangle$ with $\left|10,-\tfrac{1}{2}\right\rangle$. In total, the eight $n = 2$ states are split into five energy levels, three of which have two-fold degeneracy. - We now consider the impact of fine structure, treating H_{Z} as part of the unperturbed Hamiltonian. For simplicity, we only consider the spin-orbit contribution,

$$H_{\mathrm{SO}} = f(r)\mathbf{L}\cdot\mathbf{S}, \quad f(r) = \frac{\alpha^2}{2}\frac{1}{r}\frac{dV}{dr}$$

This is the conceptually trickiest one, since it prefers the coupled basis, while we must work in the uncoupled basis $|n\ell m_\ell m_s\rangle$, where there are two-fold degeneracies.

- Using this basis is tricky because H_{SO} can modify m_ℓ and m_s values (though not ℓ values, since $[L^2, H_{\mathrm{SO}}] = 0$). However, it can only modify m_ℓ and m_s by at most one unit at a time, since

$$\mathbf{L}\cdot\mathbf{S} = \frac{1}{2}\left(L_+ S_- + L_- S_+\right) + L_z S_z$$

or by applying the Wigner-Eckart theorem. The $2p$ degenerate states differ in m_s by multiples of 2, so H_{SO} can't mix the degenerate states. Hence to calculate the first order shift, it suffices to look at its diagonal matrix elements.

- Thus, the energy shifts are

$$\Delta E = \langle n\ell m_\ell m_s |\, f(r)\mathbf{L}\cdot\mathbf{S}\,| n\ell m_\ell m_s\rangle = m_\ell m_s \langle n\ell m_\ell |\, f(r)\,| n\ell m_\ell\rangle$$

and for hydrogen we have

$$\Delta E = m_\ell m_s \frac{\alpha^2}{2}\langle n\ell 0|\frac{1}{r^3}|n\ell 0\rangle = \frac{\alpha^2}{2n^3}\frac{m_\ell m_s}{\ell(\ell+1/2)(\ell+1)}$$

In the case $\ell = 0$, the form above is indeterminate, but the energy shift is zero by similar reasoning to before.

Normal Zeeman effect (aka strong-field, aka Paschen–Back effect) from general physics

Only atoms with a total spin angular momentum = 0 show the normal Zeeman effect.

$$E = -\mu_0 \boldsymbol{m} \cdot \boldsymbol{H}$$

$$I = \frac{ev}{2\pi a} = -\frac{|e|v}{2\pi a}; \qquad A = \pi a^2.$$

$$\boldsymbol{m} = IA = \frac{eva}{2} = -\frac{|e|va}{2}.$$

$$m_\mathrm{e} va = m_l \hbar,$$
$$v = \frac{m_l \hbar}{m_\mathrm{e} a}.$$

$$\boldsymbol{m} = -\frac{e\hbar}{2m_\mathrm{e}} m_l = -\mu_\mathrm{B} m_l.$$

$$m = \mu_\mathrm{B}\sqrt{l(l+1)},$$

$$E = \mu_0 \frac{e\hbar}{2m_\mathrm{e}} m_l H = \mu_0 \mu_\mathrm{B} m_l H.$$

$$E = \mu_\mathrm{B} m_l H.$$

$$\mu_\mathrm{B} = e\hbar/2m_\mathrm{e} \sim 9.274 \times 10^{-24}\ \mathrm{J/T} = e\hbar/2m_\mathrm{e}c = 0.927 \times 10^{-20}\mathrm{erg/Oe}.$$

$$|\boldsymbol{S}| = \sqrt{s(s+1)}\hbar = \frac{\sqrt{3}}{2}\hbar$$

$$\boldsymbol{m} = -g_\mathrm{e}\mu_\mathrm{B} m_s,$$
$$m = g_\mathrm{e}\mu_\mathrm{B}\sqrt{s(s+1)}$$

$$g_\mathrm{e} = 2.002319$$

Anomalous Zeeman effect (aka weak-field, with Lande factor) from quantum mechanics

- For hydrogen, we should properly consider the Lamb shift, which is only 10 times smaller than the fine structure shifts on the $n = 2$ energy levels. However, we will ignore it for simplicity.

- In this case, we need to use the coupled basis $|n\ell j m_j\rangle$. The difficulty is that $[J^2, H_\mathrm{Z}] \neq 0$. Luckily, the fine-structure energy levels depend directly on j, in the sense that energy levels with different j are not degenerate. Hence to calculate the first-order shift, we again do not have to diagonalize any matrices, and can focus on the diagonal elements,

$$\Delta E = \langle n\ell j m_j |\, \mu_B B \left(L_z + 2S_z\right) |n\ell j m_j\rangle$$

$L_z + 2S_z = J_z + S_z,$

$$\Delta E = \mu_B B \left(m_j + \langle n\ell j m_j |\, S_z\, |n\ell j m_j\rangle\right)$$

$$\langle n\ell j m_j|\, S_z\, |n\ell j m_j\rangle = \frac{1}{j(j+1)}\, \langle n\ell j m_j|\, (\mathbf{S}\cdot\mathbf{J}) J_z\, |n\ell j m_j\rangle$$

$$\mathbf{S}\cdot\mathbf{J} = \frac{1}{2}\left(J^2 + S^2 - L^2\right)$$

$$\Delta E = g_L\,(\mu_B B)\, m_j, \quad g_L = 1 + \frac{j(j+1) + s(s+1) - \ell(\ell+1)}{2j(j+1)}$$

Об эффекте Штарка

Типичный Штарк-эффект

В $\mathcal{E} = \{0, 0, \mathcal{E}\}$, тогда

$$\hat{\mathrm{H}} = \frac{\hat{\mathrm{p}}^2}{2} - \frac{1}{r} + \mathcal{E} r\cos\theta \equiv \hat{\mathrm{H}}^{(0)} + \hat{\mathrm{V}}, \qquad (h = m = e = 1)$$

В этой СЕ величина $\mathcal{E}$ это отношение напряженности внешнего электрического поля к внутриатомному $\varepsilon_a = e/a^2 \simeq 5,14 \cdot 10^9$ В/см.

Штарк-эффект в случае близких уровней по МК

Расщепление дублета $2s_{1/2}, 2p_{1/2}$ в слабом электрическом поле в атомных единицах равно 6δ.

Рассмотрим, например, состояния $2s_{1/2}$ и $2p_{1/2}$ атома водорода. Они обладают одинаковой энергией (если не учитывать лэмбовского смещения). Расщепление такого дублетного уровня при наложении электрического поля линейно по полю и равно $E_2 - E_1 = 2\,|V_{12}|$.

Вычислим V_{12}. Для состояния $2s_{1/2}$ волновая функция равна $R_{20}(r)\frac{1}{\sqrt{4\pi}}$, а для состояния $2p_{1/2}$ равна $R_{21}\sqrt{\frac{3}{4\pi}}\cos\theta$,

$$V_{12} = -\mathscr{E}\,(R_{20}|r|R_{21})\,\frac{\sqrt{3}}{4\pi}\int \cos^2\theta d\Omega = -\frac{\mathscr{E}}{\sqrt{3}}\,(R_{20}|r|R_{21})\,.$$

Матричные элементы динольного момента для кулоновских радиальных функций табулированы. В частности, $(R_{20}|r|R_{21}) = 3\sqrt{3}$. Следовательно, $|V_{12}| = 3\delta$.

Зависимость штарковского расщепления различных компонент мультиплетного уровня от J по Ландау пар. 76:

$$\widehat{\alpha}_{ik} = a\delta_{ik} + b\left(\widehat{L}_i\widehat{L}_k + \widehat{L}_k\widehat{L}_i - \frac{2}{3}\delta_{ik}\widehat{\mathbf{L}}^2\right)$$

$$\alpha = a, \quad \beta = b\frac{3(\mathbf{JL})[2(\mathbf{JL}) - 1] - 2J(J+1)L(L+1)}{J(J+1)(2J-1)(2J+3)}$$

(???)

The Quadratic Stark Effect

$$\Delta E = e^2\mathcal{E}^2 \sum_{n=2}^{\infty} \sum_{l,m} \frac{|\langle 1,0,0|z|n,l,m\rangle\ |^2}{E_1 - E_n}$$

$$\Delta E = -4\pi\epsilon_0 C \mathcal{E}^2 a_0^3$$

$$\mathbf{P} = -\nabla_{\mathbf{E}} E$$

$$\Delta E = -\frac{1}{2}\mathbf{P}\cdot\mathbf{E}$$

$$\mathbf{P} = 2C \times 4\pi\epsilon_0 a_0^3 \mathbf{E}$$

(дочитаю Тонга скоро!!)

(см. Ландау пар 76)

$$\widehat{V} = \frac{1}{6}\frac{\partial^2\varphi}{\partial x_i \partial x_k}\widehat{Q}_{ik}$$

Изменение времени жизни $2s1/2$ водорода в электрическом поле по МК

Время жизни состояния $2s_{1/2}$ водорода на девять порядков уменьшается при наложении электрического поля $\mathscr{E} \sim \frac{1}{x_{12}\tau} \sim \frac{1}{\tau} \sim c^{-3} \sim \frac{10}{c^9}{}^3 B \sim 500b$

В атоме водорода состояние $2s_{1/2}$ имеет большое время жизни, Действительно, переход $2s_{1_{12}} \to 1s_{1/2}$ может происходить лишь с испусканием двух γ-квантов. Время жизни состояния $2s_{1/2}$ по отношению к этому переходу порядка $1/7$ сек.

Кроме того, возможен еще дипольный переход $2s_{1/2} \to 2p_{1/2}$ (энергии обоих состояний различаются из-за лэмбовского смещения). Оценим вероятность этого перехода. В (1.4) мы нашли, что вероятность динольного перехода $w \sim \omega^3/c^3$, ω-частота перехода. Разность энергий $\omega = E_{2s_{1/2}} - E_{2p_{1/2}} \sim 1/c^3$. Следовательно, $w \sim 1/c^{12}$. В атомных единицах $c \approx 137$, следовательно, $w \sim 10^{-24}$, т. е. время жизни состояния $2s_{1/2}$ по отношению к переходу $2s_{1/3} \to 2p_{1/s}$ порядка $10^{24}\tau_{\mathbf{a}_\mathrm{T}}$, $\tau_{\mathrm{ат}}$ - атомное время $\sim 10^{-10}$ сек. Итак, рассматриваемое время $\sim 10^8$ сек. Переход $2s_{1/2} \to 1s_{1/2}$ все же вероятнее, чем переход $2s_{1/2} \to 2p_{1/2}$.

При наложении внешнего поля состояние атома будет суперпозицией состояний $2s_{1/2}$ и $2p_{1/2}$. Но как только атом перейдет в состояние $2p_{1/s}$, он моментально (за время $\tau \sim 10^{-9}$ сек) совершит дипольный переход: $2p_{1/2} \to 1s_{1/2}$. Мы видим, что время жизни состояния $2s_{1/2}$ резко изменяется при наложении электрического поля.

(потом уже коротко буду все это писать)

1.5.7 Motion in magnetic field, fundamentals of magnetism

Particle in magnetic field

Основные формулы квантового движения в магнитном поле и уровней Ландау

$$H_{\mathrm{c}}(\boldsymbol{p},\boldsymbol{r}) = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 + e\varphi(\boldsymbol{r})$$

$$\boldsymbol{v} = \boldsymbol{p} - \frac{e}{c}\boldsymbol{A}, \qquad \boldsymbol{v} = (v_1, v_2, v_3)$$

$$\{v_1, v_2\} = -\frac{e}{m^2 c} B_3, \quad \{v_2, v_3\} = -\frac{e}{m^2 c} B_1, \quad \{v_3, v_1\} = -\frac{e}{m^2 c} B_2,$$

$\boldsymbol{B} = (B_1, B_2, B_3)$ - компоненты $\boldsymbol{B} = \operatorname{curl} \boldsymbol{A}$. Таким образом, одновременно 3 компоненты скорости измерить нельзя.

$$\frac{1}{2m}\left[\left(\widehat{p}_x + \frac{eH}{c} y\right)^2 + \widehat{p}_y^2 + \widehat{p}_z^2\right]\psi - \frac{\mu}{s}\sigma H \psi = E\psi.$$

$$\psi = \exp\left[\frac{i}{\hbar}\left(p_x x + p_z z\right)\right] \chi(y)$$

$$\chi'' + \frac{2m}{\hbar^2}\left[\left(E + \frac{\mu\sigma}{s}H - \frac{p_z^2}{2m}\right) - \frac{m}{2}\omega_H^2 \left(y - y_0\right)^2\right]\chi = 0,$$

$$E = \left(n + \frac{1}{2}\right)\hbar\omega_H + \frac{p_z^2}{2m} - \frac{\mu\sigma}{s}H \qquad \text{Landau levels}$$

$\mu/s = -|e|\hbar/mc$,

$$E = \left(n + \frac{1}{2} + \sigma\right)\hbar\omega_H + \frac{p_z^2}{2m}$$

eig. f.: $\chi_n(y) = \dfrac{1}{\pi^{1/4} a_H^{1/2}\sqrt{2^n n!}} \exp\left(-\dfrac{(y-y_0)^2}{2a_H^2}\right) H_n\left(\dfrac{y-y_0}{a_H}\right)$. $\qquad a_H := \sqrt{\dfrac{\hbar}{m\omega_H}}$

(как и у осциллятора, с небольшим изменением обозначений)

Обсудим кратность уровней в магнитном поле. Поскольку $E = \left(n + \frac{1}{2}\right)\hbar\omega_H + \frac{p_z^2}{2m} - \frac{\mu\sigma}{s}H$ не содержит p_x, пробегающей непрерывный ряд значений, уровни энергии вырождены с непрерывной кратностью.

Кратность вырождения конечная, если движение в плоскости xy ограничено конечной площадью $S = L_x L_y$. Число различных (теперь дискретных) значений p_x в интервале Δp_x равно $(L_x/2\pi\hbar)\,\Delta p_x$. Допустимы все значения p_x, для которых центр орбиты находится внутри S (мы пренебрегаем радиусом орбиты по сравнению с большим L_y). Из условий $0 < y_0 < L_y$ имеем $\Delta p_x = eHL_y/c$. Следовательно, число состояний (для заданных n и p_z) есть $eHS/2\pi\hbar c$. Если область движения ограничена также и вдоль оси z (длиной L_z), то число возможных значений p_z в интервале Δp_z есть $(L_z/2\pi\hbar)\,\Delta p_z$ и число состояний в этом интервале есть

$$N_{\text{degen}} = \frac{eHS}{2\pi\hbar c}\frac{L_z}{2\pi\hbar}\Delta p_z = \frac{eHV}{4\pi^2\hbar^2 c}\Delta p_z.$$

И еще есть 2 за счет спинового выржождения.

Рассмотрим релятивистский электрон в МП, например, в графене (монослой графита):

$$\varepsilon_{\mathbf{p}} = v\sigma \cdot \mathbf{p} \qquad \sigma = (\sigma_x, \sigma_y)\,;\ \mathbf{p} = (p_x, p_y)$$

$$\varepsilon_n = \varepsilon_0\sqrt{|n|}\,\operatorname{sign}(n), \quad \varepsilon_0 = \hbar v\sqrt{\frac{2eH}{\hbar c}}, \quad (n = 0, \pm 1, \pm 2, \ldots)$$

n represents an electron-like ($n > 0$) or a hole-like ($n < 0$) LL index.

Вырождение каждого магнитного уровня по центру орбиты электрона такое же, как и для обычного спектра $\varepsilon_p = p^2/(2m)$, и равно eH$/(2\pi\hbar c)$. Плотность состояний в магнитном поле дается обычным соотношением:

$$g(\varepsilon) = \nu \frac{eH}{2\pi\hbar c} \sum_{n=-\infty}^{\infty} \delta\left(\varepsilon - \varepsilon_n\right) \qquad \nu := 2 \times 2 = 4$$

For massive Dirac fermions in a Bernal graphene bilayer, the LL spectrum takes the form

$$E_n = \pm\left\{\hbar\omega_c[n(n-1)]^{1/2} + E_g/2\right\}, \quad n = 0, 1, 2...$$

Here $\omega_c = eB/m^*$ is the cyclotron frequency, m^* is the effective mass of the quasiparticles, and E_g is the band gap. (from PHYS. REV. B 91, 115405 (2015))

Graphen's high-magnetic-field Landau level spectrum consists of almost equidistant groups of four-fold degenerate states at finite energy and eight zero-energy states. (see the article by Edward McCann and Vladimir I. Fal'ko: Landau level degeneracy and quantum Hall effect in a graphite bilayer)

Уравнение Шредингера в магнитном поле по Ландау

$$\mu_B = \frac{|e|\hbar}{2mc} = 0,927 \cdot 10^{-20} \frac{\text{эрг}}{\text{Гс}}.$$

$$\widehat{H} = \frac{1}{2m}\left(\widehat{\mathbf{p}} - \frac{e}{c}\mathbf{A}\right)^2 + e\varphi$$

$$\widehat{H} = \frac{1}{2m}\widehat{\mathbf{p}}^2 - \frac{e}{2mc}(\widehat{\mathbf{p}}\mathbf{A} + \mathbf{A}\widehat{\mathbf{p}}) + \frac{e^2}{2mc^2}\mathbf{A}^2 - \frac{\mu}{s}\widehat{\mathbf{s}}\mathbf{H} + e\varphi$$

$$\widehat{\mathbf{p}}\mathbf{A} - \mathbf{A}\widehat{\mathbf{p}} = -i\hbar \operatorname{div}\mathbf{A}.$$

$$\mathbf{A} \equiv (1/2)[\mathbf{H}\mathbf{r}]$$

$$m\widehat{\mathbf{v}} = \widehat{\mathbf{p}} - \frac{e}{c}\mathbf{A}$$

$$\{\widehat{v}_x, \widehat{v}_y\} = i\frac{e\hbar}{m^2c}H_z, \qquad \{\widehat{v}_y, \widehat{v}_z\} = i\frac{e\hbar}{m^2c}H_x \qquad \{\widehat{v}_z, \widehat{v}_x\} = i\frac{e\hbar}{m^2c}H_y$$

Атом в магнитном поле по Ландау, диамагнитная восприимчивость

$$\widehat{H} = \frac{1}{2m}\sum_a \left[\widehat{\mathbf{p}}_a + \frac{|e|}{c}\mathbf{A}\left(\mathbf{r}_a\right)\right]^2 + U + \frac{|e|\hbar}{mc}\mathbf{H}\widehat{\mathbf{S}}$$

$$\widehat{H} = \widehat{H}_0 + \mu_B(\mathbf{L} + 2\widehat{\mathbf{S}})\mathbf{H} + \frac{e^2}{8mc^2}\sum_a [\mathbf{H}\mathbf{r}_a]^2$$

$$\widehat{\mu}_{\text{ат}} = -\mu_B(\widehat{\mathbf{L}} + 2\widehat{\mathbf{S}})$$

$$\Delta E = \mu_B H\left(\bar{L}_z + 2\bar{S}_z\right) = \mu_B H\left(\bar{J}_z + \bar{S}_z\right).$$

$$\mathbf{SJ} = \frac{1}{2}[J(J+1) - L(L+1) + S(S+1)]$$

$$\Delta E = \mu_B g M_J H$$
$$g = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}$$

$$\widehat{H} = \widehat{H}_0 - \widehat{\boldsymbol{\mu}}\mathbf{H} = \widehat{H}_0 - \widehat{\boldsymbol{\mu}}_z H$$

$$\bar{\mu}_z = -\frac{\partial \Delta E}{\partial H},$$

$$\bar{\mu}_z = -\mu_B g M_J.$$

$$\Delta E = \frac{e^2}{8mc^2}\sum_a \overline{[\mathbf{H}\mathbf{r}_a]^2} = \frac{e^2}{12mc^2}H^2\sum_a \overline{r_a^2}.$$

$$\chi = -\frac{e^2}{6mc^2}\sum_a \overline{r_a^2}.$$

$$\Delta E = \mu_B H\left(M_L + 2M_S\right) + A M_L M_S$$

$$\Delta E = \mu_B g_{nJ} H M_J,$$

$$\sum_n g_{nJ} M_J = \sum_{SL} g_{SLJ} M_J \qquad \Rightarrow \qquad \sum_n g_{nJ} = \sum_{SL} g_{SLJ}$$

(??? я пока так и не понял, как эффект Зеемана на магнетизм влияет?)

Спин в переменном магнитном поле по Ландау

$$\widehat{H} = -\frac{\mu}{s}\widehat{\mathbf{s}}\mathbf{H}$$

$$\widehat{H} = \sum_a \widehat{H}_a, \quad \widehat{H}_a = -\frac{\mu}{s}\mathbf{H}\widehat{\mathbf{s}}_a$$

$$i\hbar\dot{\psi}^\nu = -2\mu\mathbf{H}\widehat{\mathbf{s}}\psi^\nu.$$

$$\begin{aligned} i\hbar\dot{\psi}^1 &= -\mu H\psi^1, & \psi^1 &= c_1\exp\left(\frac{i\mu}{\hbar}\int H dt\right)\\ i\hbar\dot{\psi}^2 &= \mu H\psi^2. & \psi^2 &= c_2\exp\left(-\frac{i\mu}{\hbar}\int H dt\right). \end{aligned}$$

$$\psi^1 = e^{-i\omega t/2}\left(c_1 e^{i\Omega t/2} + c_2 e^{-i\Omega t/2}\right),$$
$$\psi^2 = 2\omega_H \sin\theta e^{i\omega t/2}\left[\frac{c_1}{\Omega + \omega + 2\omega_H\cos\theta}e^{i\Omega t/2} - \frac{c_2}{\Omega - \omega - 2\omega_H\cos\theta}e^{-i\Omega t/2}\right],$$

$\Omega := \sqrt{(\omega + 2\omega_H\cos\theta)^2 + 4\omega_H^2\sin^2\theta}.$

Плотность тока в магнитном поле по Ландау

$$\bar{H} = \int \Psi^* \left[\frac{1}{2m} \left(\widehat{\mathbf{p}} - \frac{e}{c}\mathbf{A} \right)^2 - \frac{\mu}{s}\mathbf{H}\widehat{\mathbf{s}} \right] \Psi dV$$

$$\mathbf{j} = \frac{ie\hbar}{2m} \left[(\nabla \Psi^*)\, \Psi - \Psi^* \nabla \Psi \right] - \frac{e^2}{mc}\mathbf{A}\Psi^*\Psi + \frac{\mu}{s} c \operatorname{rot} (\Psi^* \widehat{\mathbf{s}} \Psi)$$

$$\frac{\partial \rho}{\partial t} + \operatorname{div} \mathbf{j} = 0. \qquad (\rho = e|\Psi|^2)$$

$$\frac{\mu}{s} c \operatorname{rot} (\Psi^* \widehat{\mathbf{s}} \Psi) \equiv c \operatorname{rot} \mathbf{m} \qquad \mathbf{m} := \frac{\mu}{s} \Psi^* \widehat{\mathbf{s}} \Psi = \Psi^* \widehat{\mu} \Psi$$

$$\mathbf{j}_{nm} = \frac{ie\hbar}{2m} \left[(\nabla \Psi_n^*)\, \Psi_m - \Psi_n^* \nabla \Psi_m \right] - \frac{e^2}{mc}\mathbf{A}\Psi_n^*\Psi_m + \frac{\mu}{s} c \operatorname{rot} \left(\Psi_n^* \widehat{\mathbf{S}} \Psi_m \right)$$

Magnetism fundamentals

(очень коротко в контексте теории выше укажу, пока см. запись по магнетизму)

$$E_{\text{spin}} = \mu_B B s \qquad \mu_B = |e|\hbar/2m$$

Bohr's magneton $\mu_B = |e|\hbar/2m$

(!! derivation of it!)

(other important properties)

квантовом эффекте Холла

явлениях КЭД в магнитном поле

1.5.8 Relativistic QM and QED: main models

(много разных задач, выпишу указания на них потом, в теорполе уже написана теория, разберу ее скоро)

типичных моделях

О релятивистском электроне в атоме (!!!?)

The exact fine-structure formula for hydrogen (obtained from the Dirac equation without recourse to PT) is

$$E_{nj} = mc^2 \left\{ \left[1 + \left(\frac{\alpha}{n - (j + 1/2) + \sqrt{(j + 1/2)^2 - \alpha^2}} \right)^2 \right]^{-1/2} - 1 \right\},$$

which recovers mc^2, the ordinary energy levels, and the fine structure when expanded. However, at the next order additional effects appear which are not captured by the Dirac equation, such as hyperfine structure and the Lamb shift.

Proof:

$$(P - mc)\psi(x) = 0$$

$P_0 = \frac{E}{c} + \frac{e^2}{cr}, \quad \psi(x) \equiv e^{-\frac{\mathrm{i}}{\hbar}\mathrm{Et}}\psi(\boldsymbol{r}).$

$$\times(P+mc) \qquad \Rightarrow \qquad \left\{\left(p_0 + \frac{e^2}{cr}\right)^2 - \boldsymbol{p}^2 - (mc)^2 - \boldsymbol{\gamma}\cdot\boldsymbol{p}\gamma_0\frac{e^2}{cr}\right\}\psi(\boldsymbol{r}) = 0.$$

$$-\boldsymbol{\gamma}\cdot\boldsymbol{p}\gamma_0\frac{e^2}{cr} = \mathrm{i}\gamma_5\frac{\hbar^2\alpha_{\mathrm{em}}}{r^2}(\boldsymbol{\sigma}\cdot\boldsymbol{n}) \qquad \gamma\gamma_0 = -\gamma_5\boldsymbol{\sigma},\ \boldsymbol{p}\frac{1}{r} = \mathrm{i}\hbar\frac{\boldsymbol{n}}{r^2}$$

$\boldsymbol{n} := \boldsymbol{r}/r,$

$$\left\{\frac{p^2}{2m} - \frac{E}{mc^2}\frac{e^2}{r} - \frac{\hbar^2\alpha_{\mathrm{em}}}{2mr^2}\left[\alpha_{\mathrm{em}} + \mathrm{i}\gamma_5(\boldsymbol{\sigma}\cdot\boldsymbol{n})\right]\right\}\psi(\boldsymbol{r}) = \epsilon\psi(\boldsymbol{r})$$

$[\boldsymbol{l}_\alpha, (\boldsymbol{\sigma}\cdot\boldsymbol{n})] = \mathrm{i}\epsilon_{\alpha\beta\gamma}\boldsymbol{\sigma}_\beta n_\gamma, \quad [\boldsymbol{s}_\alpha, (\boldsymbol{\sigma}\cdot\boldsymbol{n})] = \mathrm{i}\epsilon_{\alpha\beta\gamma}n_\beta\boldsymbol{\sigma}_\gamma,$

$$j = l + \sigma = \mathrm{const}$$

$$\{E, j, m, l\},$$

$\Psi_\pm(\boldsymbol{r})$:

$$\left\{\frac{p^2}{2m} - \frac{E}{mc^2}\frac{e^2}{r} - \frac{\hbar^2\alpha_{\mathrm{em}}}{2mr^2}\left[\alpha_{\mathrm{em}} \pm \mathrm{i}(\boldsymbol{\sigma}\cdot\boldsymbol{n})\right]\right\}\Psi_\pm(\boldsymbol{r}) = \epsilon\Psi_\pm(\boldsymbol{r})$$

$$\Psi_\pm(\boldsymbol{r}) \equiv a_\pm\phi_{l_+}^{j,m}(\boldsymbol{r}) + b_\pm\phi_{l_-}^{j,m}(\boldsymbol{r})$$

$$\psi(\boldsymbol{r}) \quad \xrightarrow{\mathbb{P}} \quad \gamma_0\psi(-\boldsymbol{r}) = (-1)^{l+}\begin{pmatrix} a_-\phi_{l_+^j}^{j,m}(\boldsymbol{r}) - b_-\phi_{l'_-}^{j,m}(\boldsymbol{r}) \\ a_+\phi_{l_+}^{j,m}(\boldsymbol{r}) - b_+\phi_{l_-}^{j,m}(\boldsymbol{r}) \end{pmatrix}$$

Сами спиноры $\phi_{l_\pm^{j,m}}^{j,m}$ построены согласно правилам сложения двух моментов.

Поэтому

$$\boldsymbol{l}^2\phi_{l_\pm}^{j,m} = l_\pm(l_\pm+1)\,\phi_{l_\pm}^{j,m}$$

так как оператор $(\boldsymbol{\sigma}\cdot\boldsymbol{n})$ обладает отрицательной P -четностью и его квадрат равен единице, можно выбрать фазы спиноров $\phi_{l_\pm}^{j,m}$ так, чтобы

$$(\boldsymbol{\sigma}\cdot\boldsymbol{n})\phi_{l_\pm}^{j,m} = \phi_{l_\mp}^{j,m}.$$

(?????)

Значит, этот оператор смешивает состояния $\phi_{l_\pm}^{j,m}$ в уравнении (6.32), причем матрица, соответствующая вкладу орбитального движения

$$\frac{\hbar^2}{2mr^2}\left[l^2 - \alpha_{\mathrm{em}}^2 \mp \mathrm{i}\alpha_{\mathrm{em}}(\boldsymbol{\sigma}\cdot\boldsymbol{n})\right]$$

В базисе $\phi_{l_\pm}^{j,m}$ имеет вид

$$\frac{\hbar^2}{2mr^2}\begin{pmatrix} l_+(l_+1) - \alpha_{\mathrm{em}}^2 & \mp\mathrm{i}\alpha_{\mathrm{em}} \\ \mp\mathrm{i}\alpha_{\mathrm{em}} & l_-(l_-+1) - \alpha_{\mathrm{em}}^2 \end{pmatrix} = \frac{\hbar^2}{2mr^2}A$$

$$\text{e.v.} = z = \sqrt{\left(j+\frac{1}{2}\right)^2 - \alpha_{\mathrm{em}}^2}\left(\sqrt{\left(j+\frac{1}{2}\right)^2 - \alpha_{\mathrm{em}}^2} \pm 1\right) \equiv \lambda(\lambda+1)$$

$$\delta_j := j + \frac{1}{2} - \sqrt{\left(j+\frac{1}{2}\right)^2 - \alpha_{\mathrm{em}}^2}$$

$$\lambda := j \pm \frac{1}{2} - \delta_j \equiv l_\pm - \delta_j$$

Собственные значения для верхних и нижних спиноров, очевидно, совпадают, причем коэффициенты смешивания $a_\pm$ и $b_\pm$ удовлетворяют условиям построения биспиноров с заданной четностью.

В базисе собственных векторов матрицы получаем уравнение, опять имеющее вид уравнения для нерелятивистского атома водорода

$$\left\{ \frac{p_r^2}{2m} - \frac{E}{mc^2}\frac{e^2}{r} + \frac{\hbar^2}{2mr^2}\lambda(\lambda+1) \right\} u(r) = \epsilon u(r)$$

и после аналогичных случаю скалярного поля преобразований, получаем:

$$E = \frac{mc^2}{\sqrt{1 + \frac{\alpha_{em}^2}{\nu^2}}}$$

Поэтому для заданного главного квантового числа n мы имеем двукратное вырождение по орбитальному моменту l (разные значения радиального квантового числа n_r) при фиксированном значении полного момента j, если, конечно, $n > 1$ и $n > j + 1/2$, потому что В случае равенств возможны только значения $l = 0$ и $l = j - 1/2$, соответственно, при $n_r = 0$.

$$\varepsilon_{n,l} \approx -\frac{mc^2}{2n^2}\alpha_{\text{em}}^2 \left\{ 1 + \frac{\alpha_{\text{em}}^2}{n^2}\left(\frac{2n}{2j+1} - \frac{3}{4} \right) \right\}$$

Теперь значение расшепления уровней с заданным n В зависимости от j дает прекрасное согласие с экспериментами по измерению спектров в атоме водорода.

О скалярном релятивистском электроне (!?!??!?!!?!??)

$$E = \frac{mc^2}{\sqrt{1 + \frac{\alpha_{em}^2}{\nu^2}}} \qquad \text{(Enegry of bound st.)}$$

$$\mathcal{E}_{n,l} := E - mc^2 \approx -\frac{mc^2}{2n^2}\alpha_{\text{em}}^2 \left\{ 1 + \frac{\alpha_{\text{em}}^2}{n^2}\left(\frac{2n}{2l+1} - \frac{3}{4} \right) \right\}. \qquad \text{(Enegry of the bound.)}$$

Имеем снятие вырождения по l между уровнями с заданным n. Однако, эксперимент опровергает такое расщепление, например, для уровней $2s$ и $2p$, и верный результат получается с учетом спина.

Эта энергия находится из ур. Клейна-Гордона переходом к уравнению Шредингера для нерелятивистского атома водорода, но с другим зарядом и орбитальным моментом: $e^2 \mapsto \frac{E}{mc^2}e^2$; $\quad l(l+1) \mapsto \lambda(\lambda+1) = l(l+1) - \alpha_{\text{em}}^2$.

$\mathcal{A}_0(r) = -\frac{e}{r}$, $\vec{\mathcal{A}} \equiv 0$,

$$\left\{ \left(p_0 + \frac{e^2}{cr} \right)^2 - \boldsymbol{p}^2 - (mc)^2 \right\} \Phi(x) = 0, \qquad p_0 \equiv E/c$$

$$\Phi(x) \equiv \mathrm{e}^{-\frac{1}{\hbar}Et}\phi(\boldsymbol{r}), \qquad \left\{ \frac{\boldsymbol{p}^2}{2m} - \frac{E}{mc^2}\frac{e^2}{r} - \frac{e^4}{c^2}\frac{1}{2mr^2} \right\} \phi(\boldsymbol{r}) = \frac{E^2 - (mc^2)^2}{2mc^2}\phi(\boldsymbol{r}).$$

$$\phi(\boldsymbol{r}) \equiv \frac{u(r)}{r} Y_{l,m}(\theta,\varphi); \qquad \left\{ \frac{p_r^2}{2m} - \frac{E}{mc^2}\frac{e^2}{r} + \frac{\hbar^2}{2mr^2}\left(l(l+1) - \frac{e^4}{\hbar^2 c^2} \right) \right\} u(r) = \frac{E^2 - (mc^2)^2}{2mc^2} u(r),$$

$$\alpha_{\text{em}} := \frac{e^2}{\hbar c} \qquad \epsilon := \frac{E^2 - (mc^2)^2}{2mc^2}$$

$$\left\{ \frac{p_r^2}{2m} - \frac{E}{mc^2}\frac{e^2}{r} + \frac{\hbar^2}{2mr^2}\left[l(l+1) - \alpha_{\text{em}}^2 \right] \right\} u(r) = \epsilon u(r).$$

(finish writing it!!)

Это же можно получить большими преобразованиями через ряды.
(????? see my problems section and notes from KU Leuven)

О парадоксе Клейна

(тоже очень типичная тема, 1/2 страницы на это планирую, очень коротко укажу.)

О разных моделях поля Клейна-Гордона (!?!???!?!!?!??)

(абзацы тут про каждую модель, больше словами, но также основные формулы и графики приведу. почитаю ту умную книгу про них)

Оценки в квантовой электродинамике

(тут Мигдал Крайнов, но и не только)

Нулевые колебания электромагнитного поля

Фотоэффект

Времена жизни возбужденных состояний атома

Тормозное излучение

Образование пар (!!!)

Lamb shift in QED

(?? see Vergeles, I'll write first in the note on QFT, and here there will be main results)

1.5.9 Light-matter interactions, basic quantum optics

Jaynes-Cummings model

Moving from the Schrödinger picture into the interaction picture (a.k.a. rotating frame) defined by the choice $\hat{H}_0 = \hat{H}_{\text{field}} + \hat{H}_{\text{atom}}$, we obtain

$$\hat{H}_{\text{int}}(t) = \frac{\hbar\Omega}{2}\big(\underbrace{\hat{a}\hat{\sigma}_- e^{-i(\omega_c+\omega_a)t}}_{\text{fast}} + \underbrace{\hat{a}^\dagger\hat{\sigma}_+ e^{i(\omega_c+\omega_a)t}}_{\text{fast}} + \hat{a}\hat{\sigma}_+ e^{-i(-\omega_c+\omega_a)t} + \hat{a}^\dagger\hat{\sigma}_- e^{i(-\omega_c+\omega_a)t}\big).$$

Transforming back into the Schrödinger picture,

$$\hat{H}_{\text{JC}} = \hbar\omega_c \hat{a}^\dagger\hat{a} + \hbar\omega_a \frac{\hat{\sigma}_z}{2} + \frac{\hbar\Omega}{2}\left(\hat{a}\hat{\sigma}_+ + \hat{a}^\dagger\hat{\sigma}_-\right)$$

JC model by Tong

$$H_{JC} = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & ga \\ ga^\dagger & -\omega_0 \end{pmatrix} + \hbar\omega a^\dagger a$$

$$H_n = \left(n - \frac{1}{2}\right)\omega \mathbf{1}_2 + \frac{1}{2}(\omega_0 - \omega)\,\sigma^3 + \frac{1}{2}g\sqrt{n}\sigma^1$$

$$|n_+\rangle = \sin\theta|n-1,\uparrow\rangle - \cos\theta|n,\downarrow\rangle$$
$$|n_-\rangle = \cos\theta|n-1,\uparrow\rangle + \sin\theta|n,\downarrow\rangle$$

$$\tan(2\theta) = \frac{g\sqrt{n}}{\delta}, \quad \delta = \omega_0 - \omega$$

$$E_\pm = \left(n + \frac{1}{2}\right)\hbar\omega \pm \frac{1}{2}\hbar\sqrt{g^2 n + \delta^2}$$

$$|\Psi(t)\rangle = \left[e^{-iE_- t/\hbar}\sin\theta\,|n_-\rangle - e^{-iE_+ t/\hbar}\cos\theta\,|n_+\rangle\right]$$
$$P_\uparrow(t) = \frac{g^2 n}{g^2 n + \delta^2}\sin^2\left(\frac{\sqrt{g^2 n + \delta^2}}{2}t\right)$$

Death and Resurrection:

$$|\Psi\rangle = e^{-|\alpha|^2/2}e^{\alpha a^\dagger}|0,\downarrow\rangle = e^{-|\lambda|^2/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n,\downarrow\rangle$$

$$|\Psi(t)\rangle = e^{-\left(|\alpha|^2 - i\omega t\right)/2}\sum_{n=0}^{\infty}\frac{\left(\alpha e^{-i\omega t}\right)^n}{\sqrt{n!}}\left[\cos\left(\frac{g\sqrt{n}t}{2}\right)|n,\downarrow\rangle + i\sin\left(\frac{g\sqrt{n}t}{2}\right)|n-1,\uparrow\rangle\right]$$

$$P_\uparrow(t) = e^{-|\alpha|^2}\sum_{n=0}^{\infty}\frac{|\alpha|^{2n}}{n!}\sin^2\left(\frac{g\sqrt{n}t}{2}\right)$$

$$P_\uparrow(t) = e^{-|\alpha|^2}\sum_{n=0}^{\infty}\frac{|\alpha|^{2n}}{n!}\left(\frac{1}{2} - \frac{1}{2}\cos(g\sqrt{n}t)\right) = \frac{1}{2} - \frac{1}{2}e^{-|\alpha|^2}\sum_{n=0}^{\infty}\frac{|\alpha|^{2n}}{n!}\cos(g\sqrt{n}t)$$

$$\frac{|\alpha|^{2n}}{n!} \approx \frac{1}{\sqrt{2\pi n}}e^{n\log|\alpha|^2 - n\log n + n} \overset{f''(n_{\max})=-1/n}{\approx} \frac{1}{\sqrt{2\pi|\alpha|^2}}e^{|\alpha|^2 - m^2/2|\alpha|^2}$$

$m = n - |\alpha|^2$.

$$P_\uparrow(t) \approx \frac{1}{2} - \frac{1}{2}\sum_{m=-\infty}^{\infty}\frac{1}{\sqrt{2\pi|\alpha|^2}}e^{-m^2/2|\alpha|^2}\cos\left(gt\sqrt{|\alpha|^2 + m}\right)$$

$$T_{\text{Rabi}} \approx \frac{2\pi}{g|\alpha|}$$

$gT\left(\sqrt{|\alpha|^2 + |\alpha|} - |\alpha|\right) \approx 2\pi$, or

$$T_{\text{collapse}} \approx \frac{4\pi}{g}$$

(!!! графики очень известные вставлю, см. пока хотя бы Тонга)

Rabi oscillations

$$\hat{H} = \begin{pmatrix} E_0 + \Delta & We^{-i\omega t} \\ We^{i\omega t} & E_0 - \Delta \end{pmatrix}$$

$$P_1(t) = \frac{W^2}{(\Delta - \hbar\omega/2)^2 + W^2} \sin^2\left(\frac{\Omega t}{2}\right), \quad \Omega = \frac{2\sqrt{(\Delta - \hbar\omega/2)^2 + W^2}}{\hbar}$$

coherent states

squeezing

manipulations of individual atoms;

системах с дискретными степенями свободы

Блоховское представление двухуровневой системы

взаимодействии двухуровневых систем с электромагнитным полем

$$\hat{V} = -\mathbf{dE}$$

$$\hat{V} = \hbar\Omega_R \left(\hat{a} + \hat{a}^+\right)\left(\hat{\sigma} + \hat{\sigma}^+\right)$$

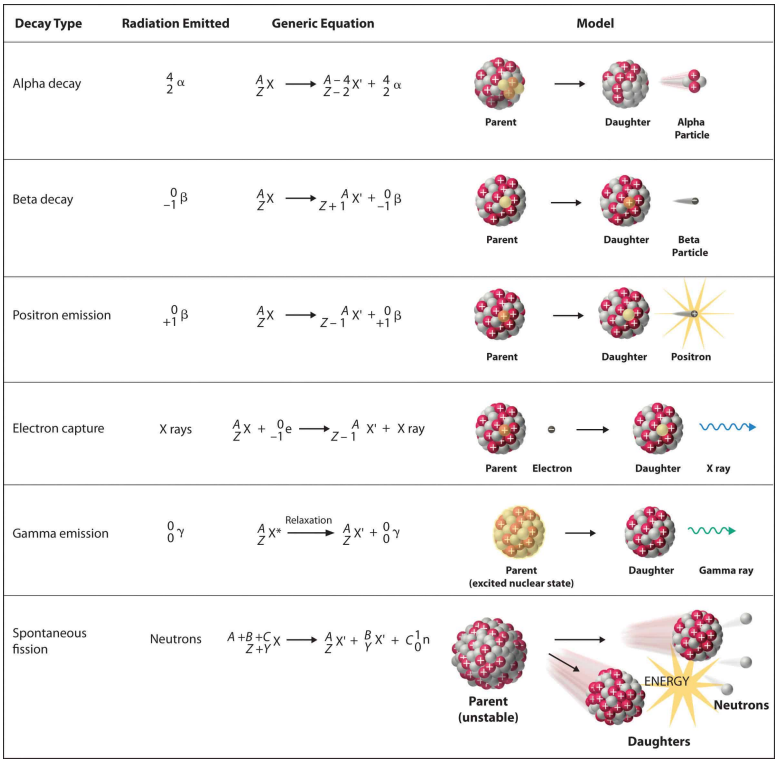
где $\Omega_R = -\left(\mathbf{E}_0\hat{\mathbf{d}}_{eg}\right)\sin\left(\frac{\omega z}{c}\right)$ - частота Раби в поле «одного фотона», поляризованного вдоль оси x. Она играет роль константы связи ДУС и МР.

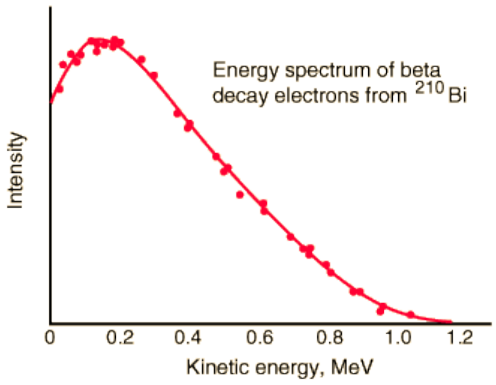
Гамильтониан Джейнса-Каммингса:

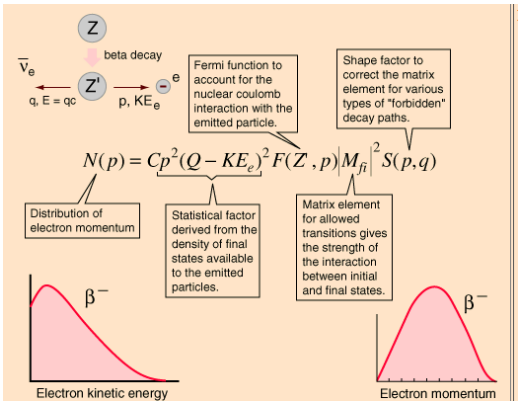
$$\hat{H} = \hbar\omega_{MP}\hat{a}^+\hat{a} + \hbar\omega_{\text{дус}}\,\hat{\sigma}^+\hat{\sigma} + \hbar\Omega_R\left(\hat{a}^+\hat{\sigma} + \hat{a}\hat{\sigma}^+\right).$$

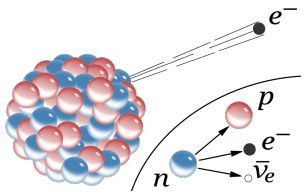
1.5.10 Nuclear physics: basic effects

(тут указания про самые основные задачи про атомы из ЛЛ3. всё остальное - во 2й 1й части, там отдельный раздел про разные модели)

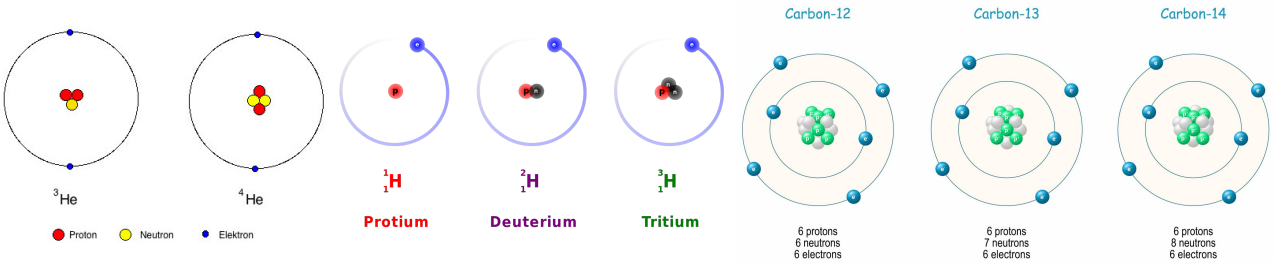




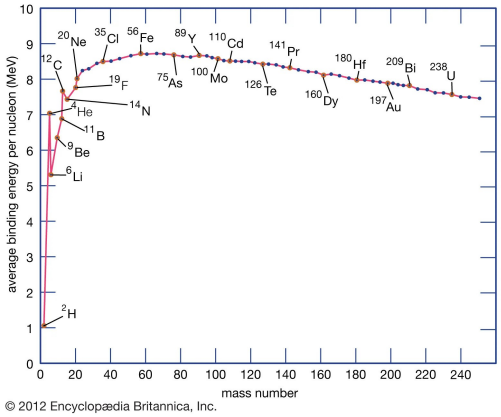




Properties of main elements



(!! I'll add main properties here!)



Ionization

(see LL3 for now)

Определение энергии ионизации

(тут всё для этой задачи!!!)

Обзор взаимодействий в атоме (???)

там есть ss, ls взаимодействия.
вот про них обзор и будет, пока нужно доучить это, задачи решить!!

Оценки в атомной механике МК

(потом впишу эти подпараграфы с оценками в структуру выше)

Оценки скоростей и размеров орбит внутренних электронов атома

Стационарные состояния

Распределение электрического заряда атоме

Неприменимость классической механики при больших прицельных параметрах (!!!!!!!)

Оценка сечения рассеяния для потенциалов, спадающих с расстояний быстрее, чем кулоновский (?????)

Резонансные эффекты при рассеянии (!!!!!)

Взаимодействие между атомами

Ионизация атомов

Многократное рассеяние

Typical β-decays (!?!?!!)

Basic nuclear phenomena by Migdal Krainov

Ионизация атомов при β-распаде (78).

Ионизация атомов при ядерных реакциях (81).

Передача энергии при вылете кванта из ядра молекулы (эффект Мёссбауэра) (83).

1.5.11 Key fundamental experiments

Об опыте Юнга

(конкретно, в каких параметрах установки он будет?)
Один из самых важнейших опытов квантовой механики, дающий пояснение, что такое суперпозиция состояний - это опыт Юнга

О влиянии наблюдателя

Никакого влияния наблюдателя нет, просто обычные волновые свойства света проявляются и все.
(потом напишу точнее, важное указание)

Об опытах, устанавливающих спектры атомов

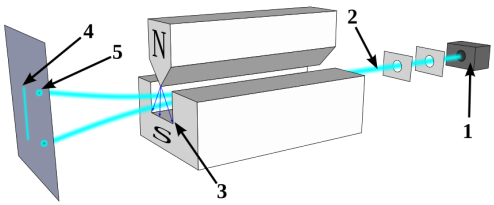
Об опыте Дэвиссона-Джермера (?)

Опыт Дэвиссона-Джермера - физический эксперимент 1927 г. по дифракции электронов.

В нем наблюдалась дифракция электронов на кристаллической решётке монокристалла.

говорят, что это с УШ связано, а также с волнами де бройля, да я хз.

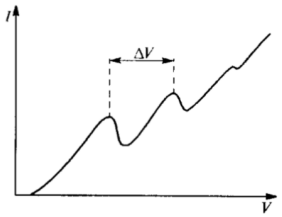
Stern–Gerlach experiment



The Franck–Hertz experiment (Nobel prize 1925)

It was the first electrical measurement to clearly show the quantum (discrete) nature of atoms.

Между катодом и анодом помещается гелий, далее увеличивая напряжение будем мерить проходящий ток. В итоге:



Proof: (??????????????)

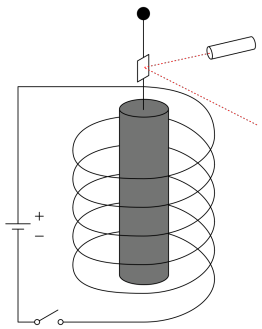
$$F = \mu_z \left(\frac{dB}{dz}\right)$$

$$V_Z = \frac{F}{m}t = \frac{F}{m}\frac{L}{V_X}$$

$$\Theta = \frac{V_Z}{V_X} = \mu_z \left(\frac{dB}{dz}\right)\frac{L}{mV_X^2} = \mu_z \left(\frac{dB}{dz}\right)\frac{L}{2T}$$

Об опыте Эйнштейна-де Гааза (????)

(???)



Об опыте Томсона?

(редко его упоминают)

Nobel experiment by Aspect, Clauser, Zeilinger

(потом дочитаю, там много думать нужно)

On other Nobel prize quantum experiments

On Lenard's experiment on cathode rays (NP 1905)

for his work on cathode rays

Part II
Fundamentals of Quantum Mechanics

Обсудим основы квантовой механики.

2 Main General Fundamentals

2.1 Experimental Facts in Basis of Quantum Mechanics

(тут коротко эксперимент - и то, как он указывает на то, почему квантмех именно так мы построили в итоге.)

This is important because our philosophy is based on observations. We can't say anything without observing nature.

2.1.1 Quantum Tunneling

Main ideas

(I'll describe this phenomena)

Some models with quantum tunneling

(???)

Tunneling bullet that hits an object

(??? what is the probability that it will just tunnel through without destroying the object? I have no idea now)

Probability of fall a standing cup

(I heard that it is also can be analyzed by quantum tunneling method... I'll write later)

Other about quantum tunneling

(???)

2.2 How In General We See Quantum World?

2.2.1 What is the Microworld And Particle?

Почему нам не хватает классической механики?

What is a particle?

(I am not sure, just a concept, it is not clear, what is it and what is meant by this question?)

Short history of concept of particle

(write about ancient times, people understood it even way before modern civilizations)

Появилось это название в 30-х годах, когда единственными представите- лями рассматриваемой группы были протон, нейтрон, электрон и фотон. Эти четыре частицы служат основой для построения окружающего нас вещества и взаимодействующего с ним электромагнитного поля и назвать их элементарными было вполне естественно.

Вначале была обнаружена первая античастица — позитрон, предсказанный П. Дираком в 1928 г. Открыт позитрон был в космических лучах в 1932 г. американским физиком К. Андерсоном (1905-2005). Эта частица отличалась от электрона только знаком электрического заряда.

Окей, классической механики не хватает, но почему вообще нам нужны именно операторы?

Философия, с которыми ожидаемо направление работы с операторами

(??? почему мы так делаем??)

Почему мы в принципе можем описывать природу операторами? (???)

(пока не знаю, что ответить, можем и все... потом напишу нормальный ответ.)

Операторы - решение проблемы?

(мб)

А как мы представляем квантовый мир и как это соотносится с базовой математикой в основе квантовой механики?

(про визуализацию обсуждение, это тоже важно, потому что часто именно из визуальной идеи мы и начинаем строить теории)

Настоящие измерительные приборы тоже квантовые

Можно ли сделать мир только квантовым, не имея вообще ничего классического, так чтобы и наблюдатель был квантовым?

(вроде как нет, классический предел и классические наблюдатели у нас всегда появляются. это фундаментальный вопрос в физике)

(то, что с Кириллом обсуждали)

Что делает теорию квантовой?

(на стак эксчендже есть тоже вопрос такой, потом подумаю.)

Какая частица элементарная?

(тоже об этом тут место написать)

Почему электрон элементарный, а протон нет?

(этот вопрос типично на КТП перекидывают, я же постараюсь тут ответить, приведя опытные факты.)

Идейно, почему и как мы можем квантовой механикой описывать кварки?

(??? не знаю, остается вопрос, там же мб другая физика, состояния связанные, хз вообще, к кваркам я всегда не готов был.)

Откуда вообще возьмется потенциал, если все массивное - волновая функция и ее взаимодействия? (!?????????????????????)

2.2.2 Connection of Classical and Quantum Mechanics

(it is not clear if one is a limit of another or not? is it indeed working? we don't need to focus on quantization here and on the formalism. There are section about answering these questions from this side later. here I want to emphasis the exactly the Connection of Classical and Quantum Mechanics and tell which views of them are wrong)

2.2.3 How Do We Understand Measurement?

Обсудим подробно идею измерений.
(с формулами - ниже раздел)

Как мы меряем параметры с фундаментальной точки зрения? (???)

Как догадаться, что следует работать с собственными значениями операторов? (!??!?!)

(да не знаю, так и не понял еще, просто пользуюсь этим и все.)

2.2.4 Planck Constant (??)

(тоже могут много вопросов появиться.)

О введении постоянной планка и перехода в предел геометрической оптики (?)

Введите универсальную постоянную Планка согласно принципу соответствия классического движения частицы пределу «геометрической оптики» для волны, допускающей описание распространения лучей согласно принципу Ферма.
(Вопросы Киселева на развлечение (?!!!!!))

Теоретически, почему она постоянная?

Экспериментально, почему она постоянная?

2.2.5 What Would Be If One Slightly Changed Fundamental Constants of QM (??)

(I'll answer these questions here, if charge e is changes, if $\hbar$ is changed, if mass of electron is changed? what would be? good questions, actually)

2.2.6 Transitions To Other Reference Frames In Quantum Mechanics (??)

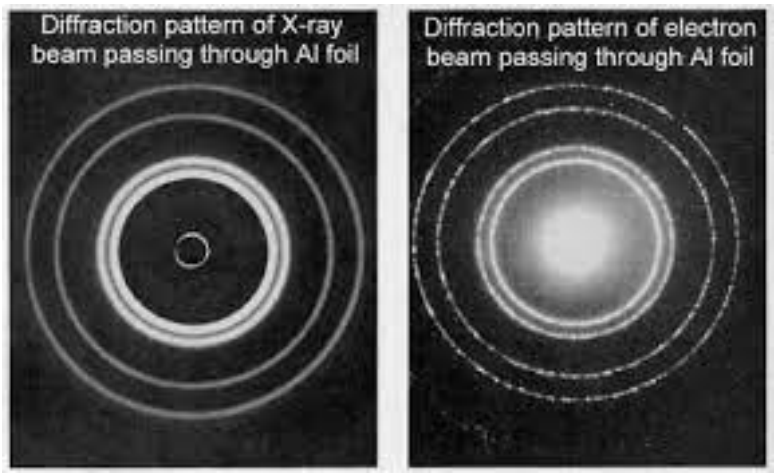
(тут же вопрос про то, как она связана с гравитацией. пока не до этого.)

Как изменится описание системы, если перейти во вращающуюся систему отсчета? (!??!!?)

(не знаю, мб много времени уйдет разобраться в этом, в механике сперва пропишу их лучше.)

2.2.7 Idea of Matter Waves

Феноменология дифракции электронов (??)



Другие свойства волн материи (????)

(есть статьи про это, пока не читал)

Волновая функция и волны материи (????)

(вроде как волновая функция даже не сразу была открыта, а уже волны какие-то материи были. так что тут про это подробнее)

О заблуждениях про волны материи

2.2.8 What Is Vacuum?

(see note on QFT, it will be first written there)

2.2.9 Wave-particle duality (?)

(тут подробно его обсуждаю)
(потом сивухина добавлю.
тут же гипотеза де Бройля: из классической механики в оптику)

Точечность частицы

Частицы всегда точечные.
(про это тут)

Почему тогда ядра не точечные?

потому что там есть нуклоны.
а почему есть нуклоны????
почему мы можем сказать, что ядра неточечные????
(остался вопрос)

Объединение корпускулярных и волновых формул в один формализм (???)

(тут формулы корпускулряных эффектов, комптон, фотоэффект)
(тут формулы волновых эффектов)
(тут общие формулы, из которых обе выше следуют.)
(??? чего еще не знаю, как это сделать???)

По киселеву

(пара слов про механику и оптику.
кстати, их отдельно тоже дописать нужно!!!) что тут типа эти вот методы нужно использовать, а не другие, там не лагранж, не еще что-то.

Из механики нам известны уравнения гамильтона, согласно которым происходит динамика нашей системы:

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q},$$

Что можно записать в виде уравнений на действие $S = \int\limits_{q_0,t_0}^{q,t} (pdq - Hdt)$, уравнений Гамильтона-Якоби:

$$\frac{\partial S}{\partial q} = p, \quad \frac{\partial S}{\partial t} = -H(q,p,t),$$

которые можно получить (да, они от туда?) из принципа наименьшего действия:

$$\delta S = 0$$

Предположим, что материя это волна, подчиняющаяся законам оптики.

Для такой волны $\Phi(q,t) \simeq e^{i\phi}$ фаза $\phi = \int\limits_{q_0,t_0}^{q,t}$ определяется принципом Ферма:

$$\delta\phi = 0$$

Если объект может быть и волной и частицей, то его динамика должна выводиться из одного и того же принципа. Поэтому, необходимо, чтобы принцип Ферма и принцип наименьшего действия были одним и тем же.

Таким образом, действие и угол должны выражаться друг через друга с помощью констант. Введем константу $\hbar$, имеющую размерность действия. Теперь волна материи может быть записана как

$$\Psi(q,t)_{\text{geom.optic}} \cong e^{\frac{i}{\hbar}S(q,t)}$$

И из этого следуют с одной стороны динамика с точки зрения механики, и волновые свойства.

теперь следствия (?это следствия?)

классические результаты де Бройля:

$$\lambda = \frac{2\pi}{k} = \frac{2\pi\hbar}{p}$$

(2.10 задача, потом додумаю)

удивительно, но соотношение де бройля позволяет определить относительные показатели преломления.

$$n = \frac{\lambda_1}{\lambda_2}$$

суть в том, что мы для частиц начинаем писать все то же, что мы писали для волн!!!

удивительно!

таким образом из энергии сразу получаемся длина волны: $\lambda = \frac{2\pi\hbar}{\sqrt{2mE}}$.

так что похоже что все наши волновые знания через де Бройля нами и будут пользоваться.

еще тут есть важные трюки с переходом к $\Delta\lambda$ и другим, это ниже разберем.

(и намеки на волновую функцию, введение в которую будет дальше)

дальше

$$\hat{p}_q \Psi(q,t) = \frac{\partial S(q,t)}{\partial q}\Psi(q,t) \cong -i\hbar\frac{\partial}{\partial q}e^{\frac{i}{\hbar}S(q,t)} \cong -\mathrm{i}\hbar\frac{\partial}{\partial q}\Psi(q,t)$$

$$\hat{p}_q = -\mathrm{i}\hbar\frac{\partial}{\partial q}$$

$$\frac{\partial S}{\partial t}\Psi(q,t) \cong -\mathrm{i}\hbar\frac{\partial}{\partial t}e^{\frac{1}{\hbar}S(q,t)} \cong -\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(q,t)$$

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(q,t) = \hat{H}\left(q,\hat{p}_q,t\right)\Psi(q,t)$$

Электроны также могут описываться волной

(напишу это красиво, это удивительно вообще)

Любая материя также может описываться волной

(напишу это красиво, это удивительно вообще. хотелось бы формулу, какого размера объекты могут описываться волной?

2.2.10 Why Do We Need Exactly a Density of Probability?

(a detailed answer is here. at first studying it is better not to think about it, just use the formalism)

2.2.11 How Do Interactions Occur?

(?? не уверен в ответе, но мы описыаем просто новым членом вз-я в гамильтониане)

How to write an interaction term of atom and field?

Why for atom interaction with electric field is $\hat{V} = eE\hat{x}$?

(Это из теории поля, где разложения. См. ЛЛ3, там подробно обсуждаются вопросы вз-я атома и поля)

Нетривиальный факт, что + и - от электрона и протона учитываются именно как дипольный момент и поэтому мы имеем дипольное взаимодействие с электрическим полем.

Квадрупольные взаимодействия иногда тоже рассматриваются, например, в сверхтонкой структуре.

Can an electron interact with its own electric field?

This is something that has been considered for a long time, even before quantum theory, people tried to see if the electron's self energy could explain its mass. Unfortunately, such calculations always yield infinity for the self-energy, unless you make some assumptions about having a finite cutoff radius, which is not observed.

However, the issue reared up again in quantum electrodynamics. The electron's own electric field is made up of photons emitted from the electron itself, and the electron can absolutely interact with such photons, these are among the terms that appear in the standard perturbation theory calculations. And just as before, these types of interaction terms are infinite in size. And it was not understood for many years what to do with this result, until Feynman and Schwinger showed how to "renormalize" the parameters of the model to absorb these infinite contributions into the model parameter definitions. The procedure leaves people uneasy, but it works extremely well, and this model, Quantum Electrodynamics is now the most accurate model of anything, anywhere, ever in human history.

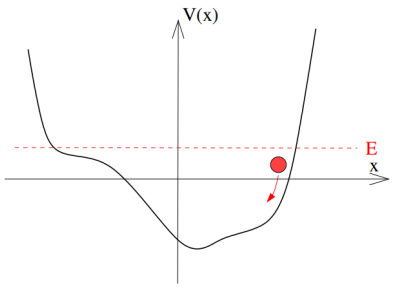
(потом продумаю!!!)

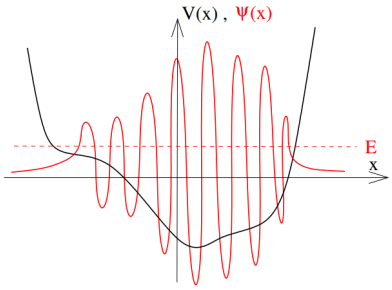
2.3 Concepts That Are Used in QM Models

2.3.1 The Main Idea of Quantum Mechanics

(тут то, что дальше во всей теории мы и применяем, с нее все и начинается.)

Сравнение классического и квантового (??)





казуальная неопределенность (??)

Подобные вероятностные характеристики имеют совершенно иную природу, не связанную с природой погрешностей прибора.

Другими словами, распределение положения точки регистрации частицы в приборе, если частица двигалась до этого свободно, без взаимодействия с системой, является распределением случайной величины, значение которой никак казуально не предопределено на каждой отдельной траектории.

Неопределённости этой случайной величинь - это новый эффект, который требует адекватного описания.

С точки зрения проблемы начальных условий следует признать, что для свободной частицы задать её координату в начальный момент времени означает задать исходную точку частицы в приборе, а значит, взаимодействие частицы с прибором должно исходно быть не равно нулю!

Напротив, в случае, если частица совершенно точно находится в заданной точке пространства, отсутствуют какие-либо данные о траектории в других точках пространства, то есть совершенно неопределено, с какой скоростью движется частица, поскольку для определения скорости необходимо получить данные о сдвиге частицы в другую точку.

Значит, если на частицу начинают действовать внешние силы, т.е. она взаимодействует с окружающей средой, положение частицы уже может быть более определенно, поскольку силы изменяют скорость частицы, то есть от них зависит сравнение характеристик движения в разных точках, но так как это положение ещё имеет ненулевую неопределённость, то и значение сил задаётся неоднозначно, силы при повторных опытах имеют флуктуации, что делает траекторию несколько неопределённой, а не абсолютно точной.

Мы видим, что неопределённости в значениях скорости и координаты частицы каким-то образом связаны казуально, но эта связь в области применимости классической механики может быть пренебрежимо малой, она существенна в квантовой механике.

В связи с вышесказанным разумнее перейти от описания эволюции системы (в данном случае, речь идёт об эволюции свободной частицы) с заданными исходными данными к описанию эволюции с заданными координатами на концах траектории: измерять координаты частицы действительно можно с любой инструментальной погрешностью.

Для свободной частицы, в отсутствие всяких сил, существуют инерциальные системы огсчёта (о них мы ещё будем разговаривать в II. 1.6), в которых частица движется поступательно и равномерно, то есть траектория является прямой линией.

В этом простейшем случае, очевидно, переход от начальных условий к данным на концах траектории является взаимно однозначнът.

При наличии сил переход к данным на концах траектории также будет взаимно однозначным, если рассматривать движение на бесконечно малом промежутке времени $t_1 - t_0 \mapsto dt \to 0$. Это справедливо и для траекторий на конечных отрезках времени, если в системе нет сингулярностей или особых симметрий.

Все другие «траектории», то есть функции $x(t)$ с теми же данными на концах не будут удовлетворять уравнениям движения с заданными начальными условиями.

Траектории, не являюшциеся решением уравнений движения, можно трактовать как траектории с другим набором сил, что влечёт за собой, конечно, и соответству ющщие изменения начальных условий, а именно, скорости в исходной точке.

В этом смысле, траектория, которая мало отличается от решения уравнений движения в заданной физической системе с фиксированными концами, получается за счёт малой флуктуации сиЛ.

Траектории с фиксированными концами: $x\left(t_0\right) = x_0, x\left(t_1\right) = x_1$, можно поставить в соответсвие число, равное единице, если эта траектория $x(t)$ является решением уравнений движения [1] в заданной физической системе, и нуль, если траектория $\bar{x}(t)$ не является решением уравнений движения.

Сконструированное нами сейчас соответствие называют динамическим функционалом достоверности траектории С:

$$\mathcal{C}[x(t)] = 1, \quad \mathcal{C}[\bar{x}(t)] = 0$$

Ясно, что при наличии нескольких частиц, которые движутся под воздействием внешних сил, динамический функционал достоверности всей системы частиц является произведением динамических функционалов достоверности для отдельных частиц:

2.3.2 Time in QM: Main ideas

(there are a lot of statements about the time, but they will be written at the last part of the note. here, there will be the most important statements)

2.3.3 Reference Frames in QM

(to know in which frame we are, we need to have photons that are coming in, but in there are a lot of models that state that something is moving, but there are no photons in that model. so, there are questions about the validity in general of these solutions. these questions I'll describe here.)

2.3.4 Idea of Operators in Quantum Mechanics

(чисто то, что используем в задачах, математика и дополнения все - в другой части.)

Суть гейзенберговского представления (???)

(укажу тут его)

The idea of spin models

(here, I'll answer this question that we have a w.f. in QM, but then later in many particle physics there are just states and action on them with on-site operators. why??? why we are so far away from Scrodinger equation??? or it is there, just the notation is fully different??)

2.3.5 Space of States (??)

Обсудим подробно пространство состояний.

2.3.6 Concept of Path Integral (??)

(intro to this method. see later parts for now with technical description of this method, or a special note about it)

2.4 Advanced General Understanding of Quantum Mechanics

$$\mathcal{C} = \prod_{i=1}^{n} \mathcal{C}_i$$

Вспомним, однако, про наличие погрешности измерения наблюдаемых характеристик частицы.

Как уже было сказано раньше, если начальные условия для координаты и скорости частицы принимают центральные значения с конечной погрешностью, то траектории из такой малой области начальных условий на малых интервалах времени будут мало отличаться от центральной траектории.

В этом случае вся «трубка» траекторий из исходной области начальных данных является эквивалентной в рамках погрешности измерений, так что для всего пучка динамический функционал достоверности траекторий в пучке равен единице.

Тем не менее, представим теперь себе ситуацию, когда

центральное значение начальных условий немного сдвинуто так, чтобы при заданной погрешности новая область начальньгх данных лишнь наполовину перекрывается с исходной областью начальных условий при той же погрешности.

Тогда динамический функционал достоверности траекторий в половине случаев принимает значение, равное единице, если траектория находится в пересечении двух областей данных, и равное нулю, если траектория находится вне исходной «трубки» траекторий.

В этом случае естественно говорить уже не о динамическом функционале достоверности траектории, а о функционале вероятности достоверности траектории $\mathcal{W}$, а в приведённом примере можно положить эту вероятность равной $\mathcal{W} = \frac{1}{2}$. Более формально, необходимо взять N_0 траекторий в области погрешности определения начальной координаты и начальной скорости и вычислить, сколько из этих траекторий попали в область фиксированных значений координаты и скорости на конце траектории N_1 за фиксированный интервал времени, и определить вероятность в зависимости от отношения $\frac{N_1}{N_0}$.

Таким образом, в общем случае, при наличии ненулевой погрешности измерений координат и скорости следует ввести функционал вероятности достоверности траектории со значениями во всем спектре от нуля до единицы: $\mathcal{W} \in [0, 1]$. Эта вероятность достоверности достигает своего максимума на решении уравнений движения с фиксированными концами траектории в заданной физической системе, то есть $\mathcal{W}$ имеет экстремум на «прямой» траектории [1]. По построению, функционал вероятности достоверности траекторий вычисляется как произведение вероятностей для независимых подсистем и подтраекторий:

$$\mathcal{W} = \prod_{i=1}^{n} \mathcal{W}_i$$

Здесь следует сделать следующее замечание: рассмотрение вероятности достоверности траекторий $\mathcal{W}$ для системы из двух тождественных частиц может привести к противоречию с принципом запрета Паули. Чтобы этого не происходило, вводится комплексная амплитуда вероятности Ψ согласно

$$\mathcal{W} = |\Psi|^2$$

При этом очевидно, что амплитуда вероятности достоверности траектории, как и сама вероятность, имеет экстремум на «прямой» траектории.

Значит, и логарифм [3] амплитуды имеет экстремум на «прямой» траектории.

Разбивая «прямую» траекторию на полтраектории, получаем

$$\ln \Psi = \sum_{i=1}^{n} \ln \Psi_i$$

Введём понятие действия S как аддитивного функционала на траектории,
пропорционального логарифму амплитуды вероятности

$$S[x(t)] = -\mathrm{i}\hbar \ln \Psi, \quad S = \sum_{i=1}^{n} S_i$$

Разбивая бесконечно малый интервал эволюции на два отрезка эволюции $dt_{12} = dt_1 + dt_2$, в силу аддитивности функционала действия находим, что $dS_{12} = dS_1 + dS_2$. На бесконечно

малом интервале действие зависит от одних и тех же значений координаты и скорости, так что при произвольном разбиении интервала условие: $dS_{12} = dS_1 + dS_2$ может быть удовлетворено, только если

$$dS = L(x, \dot{x}, t)dt$$

где функция Лагранжа $L(x, \dot{x}, t)$ зависит от определения динамических свойств физической системы.

В итоге, функционал действия на траектории задаётся в виде интеграла

$$S[x(t)] = \int_{t_0,x_0}^{t_1,x_1} L(x, \dot{x}, t)dt$$

Причём, как мы установили, на траектории, удовлетворяющей уравнениям движения, действие экстремально.

Это утверждение и составляет суть принципа экстремального действия Гамильтона, из которого мы в п. 1.3 получим уравнения движения - т.н. уравнения Эйлера-Лагранжа - для частицы (в общем случае, механической системы) с лагранжианом $L(x, \dot{x}, t)$.

2.4.1 The Limit of Healthy Philosophy of QM (??)

There are a lot of philosophers who propose to read their big books about some abstract questions in QM, listen to seminars, where they give strange statements, which are useless in a sense that one would work with QM without any problem without understanding of them. This is not the “real understanding”, which was initially proposed. Here, we will discuss this boundary between important fundamental question and waste of time, which is proposed as something very important. And this is the very big problem of quantum mechanics, one can just start thinking about such philosophical questions and come shortly to the stage when he would not be able to solve absolutely any problem. This would be just a catastrophe, so it is important to understand, which questions of QM one should postpone for a long time?

(similar things are written shortly in the section "tips for learning QM in the appendix", but here, there are informative statements about QM, and in that section, there is a focus on advice for learning)

2.4.2 Einstein’s Quantum Thought Experiments

(там как минимум на википедии есть список их, вот и обсужу их, пока не до этого)

2.4.3 Why There are Complex Numbers in QM?

(I’ll discuss this useless but interesting for a waste of time question... later!)

2.4.4 Determinism (??)

(тут про нее, уже в другом месте писал про это.)

2.4.5 Experiments, at which quantum mechanics breaks? (???)

(the most important question of quantum mechanics. since life is more than lifeless mechanics, but at what stage it emerges?)

2.4.6 At Which Point Does Lifeless Micromechanics Fail? (???)

(the most important question of quantum mechanics. since life is more than lifeless mechanics, but at what stage it emerges?)

2.4.7 Schrodinger's Cat

(I don't think that it is that important, but okay, it is a nice, fundamental topic and I still need to write it better)

2.5 Features of Interpretations of Fundamental Experiments in QM

2.5.1 Can the photoelectric effect be explained without photons?

see https://physics.stackexchange.com/questions/68147/can-the-photoelectric-effect-be-explained-without-photons, I'll think later.

2.6 Limits of Applicability of Quantum Mechanics

2.6.1 Limits of Applicability Due to Relativistic Effects

(???? write it??? if we increase speed of particles, when do we need to use different spectrum and when QM is at all not applicable?)

2.6.2 Limits of Applicability Due to Size of a System

(???? write it??? if we increase size of a system, when other effects start to play a role and when QM is at all not applicable?)

2.7 Operators, Wave Functions, States

2.7.1 Wave Function

Обсудим подробно, что такое волновая функция.

Смысл волновой функций и траектории квантового движения (!!!)

Хотя мы всегда видим только одну траекторию, никто нам не говорил, что вне измерений будет движение тоже по одной определенной траектории

как конкретно это происходит?

Что за движение частицы в точку, где она измерена, из всех точек, где ее вероятность ненулевая?

(Это звучит как самая бредовая формула в физике, но когда обсуждают смысл волновой функции, то такую формулу пишут. Тут важное обсуждение этого момента)

Свойства волновой функции

Представления волновой функции и ψ вне зависимости от представления? (?????)

Как так может быть, что есть ψ, $\psi(p)$, $\psi(x)$?
(задал этот вопрос Филиппову, так и не помню ответ, потом пропишу)
(скоро напишу ответ, но не сейчас)

That stupid notation $|\psi\rangle(x)$

(here, I'll answer, what is meant by it???? a very confusing notation)

Вероятность по волновой функции

(напишу потом, типа просто квадрат модуля. однако если у нас есть переходы, то можно брать просто скалярное произведение двух состояний, что часто делается в задачах. все, так этим и пользуюсь.)

Энергия из волновой функции (????)

(?? как это получить?)

Другие физические параметры из волновой функции

(пока не знаю.)

Нормировка волновой функции (???)

(мб сделаю большим разделом, пока лишь надеюсь, что такого раздела уже должно хватить.)

связь непрерывного и дискретного спектров через нормировку в ящике (???)

(пока хз, зачем это, потом разберу когда-то)
в итоге объем, граничные условия Борна-Кармана...

$$\psi_{\boldsymbol{p}}(\boldsymbol{r}) = \frac{1}{\sqrt{V}} e^{i\boldsymbol{p}\boldsymbol{r}}$$

хз, почему

$$\sum_{\boldsymbol{p}} \leftrightarrow \int \frac{V d^d \boldsymbol{p}}{(2\pi)^d}$$

ну и если я дойду, я начну на самом деле глубоко физику понимать.
например, можно понять, почему

$$\delta(\boldsymbol{r} - \boldsymbol{r}') \equiv \sum_{\boldsymbol{p}} \psi^*_{\boldsymbol{p}}(\boldsymbol{r}')\, \psi_{\boldsymbol{p}}(\boldsymbol{r}) \approx \int \frac{V d^d \boldsymbol{p}}{(2\pi)^d} \frac{1}{V} e^{i\boldsymbol{p}\boldsymbol{r} - i\boldsymbol{p}\boldsymbol{r}'} = \int \frac{d^d \boldsymbol{p}}{(2\pi)^d} e^{i\boldsymbol{p}(\boldsymbol{r} - \boldsymbol{r}')} = \delta(\boldsymbol{r} - \boldsymbol{r}')$$

Нормировка в случае непрерывного спектра на дельта-функцию (!?!??)

(!?!?!?? тут подробно про это напишу, важный раздел!!!)

Как и в дискретном случае, состояния, соответствующие различным собственным числам, по-прежнему ортогональны, однако они часто ненормируемы.

В непрерывном случае нормировка имеет вид: $\langle\psi_f|\psi_{f'}\rangle = c(f)\delta\left(f - f'\right)$, коэффициенты $c(f)$ могут быть любыми

Сама волновая функция через компоненты представляется

$$|\Psi\rangle = \int d\nu|\nu\rangle\Psi_\nu = \int d\nu|\nu\rangle\langle\nu|\Psi\rangle$$

Коэффициенты в общем случае можно было бы посчитать приведением скалярного произведения к виду дельта функции на коэффициент, но так никто не знает, как сделать, так что.

В данном случае нормировочные множители считаются с помощью асимптотического вида функции.

Введём произвольный масштаб λ и запишем перекрытие следующим образом

$$\int\limits_{-\infty}^{\infty} dx\psi^*_{f'}(x)\psi_f(x) = \int\limits_{-\infty}^{-\lambda} dx\psi^*_{f'}(x)\psi_f(x) + \int\limits_{\lambda}^{\infty} dx\psi^*_{f'}(x)\psi_f(x) + \int\limits_{-\lambda}^{\lambda} \psi^*_{f'}(x)\psi_f(x)dx$$

Из этого можно сделать какие-то выводы.

короче говоря, тут сказан какой-то метод про нормировку состояний непрерывного спектра, суть в том, что в разложение выше нужно подставить явный вид волновых функций, дальше выносим что угодно, что будет регулярным, так как ответ мы знаем, что он будет сингулярным.

Теперь вероятность величины быть в каком-то интервале имеет вид

$$\hat{\mathbb{P}}\left(f_1 \leq f \leq f_2\right) = \int\limits_{f_1}^{f_2} \frac{df}{c(f)}|f\rangle\langle f|$$

Плотность вероятности:

$$\rho(f)df = \langle\psi|f\rangle\langle f|\psi\rangle\frac{df}{c(f)} = |\psi(f)|^2\frac{df}{c(f)}$$

разбиение единицы имеет вид: $\hat{\mathbb{I}} = \int \frac{df}{c(f)}|f\rangle\langle f|$

В итоге наши переходы в представления делаются следующим образом:

$$\begin{cases} \psi(p) \equiv \langle p|\psi\rangle = \int dx\langle p|x\rangle\langle x|\psi\rangle \equiv \int dx e^{-ipx/\hbar}\psi(x) \\ \psi(x) \equiv \langle x|\psi\rangle = \int \frac{dp}{2\pi\hbar}\langle x|p\rangle\langle p|\psi\rangle = \int \frac{dp}{2\pi\hbar}e^{ipx/\hbar}\psi(p) \end{cases}$$

Для непрерывного спектра требования зануления одного из коэффициентов нет, из-за чего состояния непрерывного спектра двукратно вырождены

Все ли хорошо с теорией, в которой нормировка на дельта-функцию?

(?? пока вопрос остался.)

Другие свойства волновой функции

Сепарабельность и волновая функция (????)

Сепарабельность и полнота (??)

A2. Сформулируйте понятие сепарабельности и полноты пространства квантовых состояний.

Связь с квантовым полем (??)

(пока остался вопрос, ктп нужно учить)

Потенциал от волновой функции (???)

Допустим, частица описывается какой-то волновой функцией. Какой потенциал она создает для других частиц???
(не знаю, оставшийся вопрос.)

Примеры волновых функций

(из задач добавлю некоторые формулы, что типа такой потенциал например - такая функция! не вижу смысла делать структуру тут, это кругозорный параграф)
Например, волновая функция может выглядеть так:

$$\psi \propto e^{\pm ikx},$$

(где в каком-то случае $k = \sqrt{\frac{2Em}{\hbar^2}}$ (?))
Или например так:
(???)
Вот кстати их графики, чтобы прямо наглядно это представлять:
?????
а вот примеры дискретного случая:
Волновая функция свободной частицы имеет вид волны де Бройля:

$$\Psi_p(r,t) = e^{\frac{\mathrm{i}}{\hbar}(p\cdot r - Et)}$$

Общие интуитивные соображения, почему она такая, следующие:
(??)
Также ее можно найти с помощью оператора импульса, так как его действие на искомую известно:

$$\begin{aligned}\langle \boldsymbol{r}|\hat{\boldsymbol{p}}|\boldsymbol{p}\rangle &= \langle \boldsymbol{r}|\boldsymbol{p}|\boldsymbol{p}\rangle \\ \hat{\boldsymbol{p}}\Psi_{\boldsymbol{p}}(\boldsymbol{r}) &= \boldsymbol{p}\Psi_{\boldsymbol{p}}(\boldsymbol{r}) \\ -\mathrm{i}\hbar\boldsymbol{\nabla}\Psi_{\boldsymbol{p}}(\boldsymbol{r}) &= \boldsymbol{p}\Psi_{\boldsymbol{p}}(\boldsymbol{r}) \\ \Psi_{\boldsymbol{p}}(\boldsymbol{r}) &= \mathcal{N}e^{\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}\end{aligned}$$

Равенство константы $\mathcal{N} = 1$ видно из нормировки: $\langle p'|p\rangle = (2\pi\hbar)^3\delta(p'-p) \leftrightarrow \mathcal{N}^2\int d^3r e^{\frac{\mathrm{i}}{\hbar}(p-p')\cdot r} = (2\pi\hbar)^3\delta(p'-p)$.
пример: свободная частица и волны у нас

$$\hat{H}_0 = \frac{\hat{\boldsymbol{p}}^2}{2m}$$

наблюдаемы (?)

$$\hat{\boldsymbol{p}}|\boldsymbol{p}\rangle = \boldsymbol{p}|\boldsymbol{p}\rangle, \quad \hat{H}_0|\boldsymbol{p}\rangle = \frac{\boldsymbol{p}^2}{2m}|\boldsymbol{p}\rangle$$

получили что-то заумное

$$|\boldsymbol{p}'\rangle = \int |\boldsymbol{p}\rangle \frac{d^3p}{(2\pi\hbar)^3} \langle \boldsymbol{p}|\boldsymbol{p}'\rangle$$

спустя какой-то херни

$$\langle \boldsymbol{r}|\hat{\boldsymbol{p}}|\boldsymbol{p}\rangle = \langle \boldsymbol{r}|\boldsymbol{p}|\boldsymbol{p}\rangle \quad \leftrightarrow \quad \hat{\boldsymbol{p}}\Psi_{\boldsymbol{p}}(\boldsymbol{r}) = \boldsymbol{p}\Psi_{\boldsymbol{p}}(\boldsymbol{r}) \quad \leftrightarrow$$
$$-\mathrm{i}\hbar\boldsymbol{\nabla}\Psi_{\boldsymbol{p}}(\boldsymbol{r}) = \boldsymbol{p}\Psi_{\boldsymbol{p}}(\boldsymbol{r}) \to \Psi_{\boldsymbol{p}}(\boldsymbol{r}) = \mathcal{N}e^{\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}$$

имеем

$$\Psi_{\boldsymbol{p}}(\boldsymbol{r}) = e^{\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}$$

вроде это волны де бройля.
потом вернусь к этому.
и потом выводы запишу.

О представлениях волновых функций (???!)

(напишу, что такие-то есть они, чтобы потом не было удивительно, что такое вообще есть)

Координатное

Импульсное

Гейзенберга координатное или импульсное

Взаимодействия

Энергетическое, операторы рождения и уничтожения

(?? кроме осциллятора это можно еще где-то ввести??)

О возможностях других представлений?

(?? оставленный вопрос, могут ли быть еще представления и как их придумать, если нужно будет.)

О волновой функции фотона или аналоге (????)

(пока думаю, что фотон ей не описывается, ну и ладно, потом напишу четко, как вместо этого можно описывать)
Связь волновой функции фотона и интенсивностью поля от него (??)

Is the concept of a wave function applicable for photons?

(maybe no, since there is QFT for it, but I don't have a good answer yet)

Детали о волновой функции

О потенциале от волновой функции (?????)

Допустим, есть две частицы. Мы говорим, что одна описывается волновой функцией в потенциале, который создается всем вокруг. Тогда если у нас есть две частицы, то ожидаемо, что они создадут тоже потенциал друг для друга. Вопрос: как так, что волновая функция создает потенциал для других частиц? Такого свойства мы не знали.

(????? не знаю ответ на этот вопрос, напишу потом)

О регулярности волновой функции в точке с особенностью потенциала

В действительности, требование на связанные состояние накладывается одно - а именно, функция в нуле (да и вообще везде) должна быть интегрируема. Это исключает возможность иметь степенные сингулярности (которые имеют функции $Y_m(z)$ и $H_m^{(1,2)}(z)$ при $m > 0$), но не исключает возможность иметь лишь логарифмическую особенность (которая имеется при $m = 0$). Аргумент, по которому эту логарифмическую особенность нужно отбросить, немного иной. С физической точки зрения поскольку потенциал в нуле вполне себе регулярен, то было бы как минимум странно иметь там сингулярность волновой функции. Математически же это связано с тем, что $\nabla^2 \ln \frac{1}{r} = 2\pi\delta(r)$ - поэтому функция Неймана, в действительности, решает задачу о двумерной дельта-яме. В исходном потенциале такой сингулярности нет, и именно по этой причине мы можем отсеять $Y_m(z)$ также и при $m = 0$.

Что происходит с волновой функцией частицы, когда она распадается на две частицы? (?????)

(напишу потом внятный ответ на этот вопрос.)

Фундаментально материя описываются квантовым полем, или волновой функцией??

(?? напишу с формулами ответ на этот вопрос, мб как раз частный случай квантового поля - случай с одной частицей?? тут основы КТП нужно знать.)

О заблуждениях и других пониманиях волновой функции

Интерпретации квантовой механике, коллапаса функций - все это в другом разделе, тут обсуждения разных соображений про то, что такое именно волновая функция.

Что может иметься в виду под несуществующими параметрами, схожими с волновой функцией?

(лень писать, ну не понимают многие это, ну и живут, просто пользуясь формулами иногда и все)

О поверхности электрона

Об электронном облаке

О шарообразности частиц

Об неверности идеи перехода многим траекториям одновременно

(типа по одной переход происходит, просто какой конкретно - разная вероятность. напишу потом)

2.7.2 Entanglement and Purity of States (??)

Обсудим подробно принцип суперпозиции.

Чистые / факторизованные

Чистые могут быть перепутанными или не перепутанными.
Чистые не перепутанные:

$$\psi_{AB} = \psi_A \otimes \psi_B$$

$$\rho_{AB} = |\psi\rangle\langle\psi| = |\varphi\rangle\langle\varphi| \otimes |\xi\rangle\langle\xi|$$

$$\rho_{AB} = \rho_A \otimes \rho_B$$

Чистые перепутанные:

$$\psi_{AB} \neq \psi_A \otimes \psi_B$$

$$\psi_{AB} = |\psi\rangle\langle\psi| \neq |\varphi\rangle\langle\varphi| \otimes |\xi\rangle\langle\xi|$$

здесь нет вообще корреляций.
(???!!! примеры??!!!)

Смешанные состояния

Смешанные не перепутанные:

$$\rho_{AB} \neq |\psi\rangle\langle\psi|$$

$$\rho^{AB} = \sum_k p_k \rho_k^A \otimes \rho_k^B,$$

где p_k - коэффициенты в выпуклой сумме.
(???!!! примеры??!!!)

сепарабельные / распутанные / не запутанные / состояния

Физический смысл незапутанных состояний в том, что если у нас есть физическая величина, состоящая из тензорного произведения величины одной части системы F и величины второй части системы G есть произведение их средних значений

$$\langle F \otimes G\rangle = \langle F\rangle \cdot \langle G\rangle.$$

Кстати, если было бы перепутанное, то $\langle F \otimes G\rangle \neq \langle F\rangle \cdot \langle G\rangle$, то ест были бы корреляции.

Другими словами, можно брать произведение результатов.

(там что я измеряю X, коллега измеряет У, мы перемножаем их и считаем матожидание)

Проверка сепарабельности делается следующими способами.
Критерий Переса-Городецких:

$$\rho_{AB}^{T_B} \geq 0 \quad \Longrightarrow \quad \text{сепарабельно}$$

$$\rho_{AB}^{T_B} \geq 0 \quad \underbrace{\Longleftarrow}_{dimH_A \cdot dimH_B \leq 6} \quad \text{сепарабельно}$$

В частности для двух кубитов, критерий Переса-Городецких утверждает, что их матрица плотности является сепарабельной тогда и только тогда, когда она остается матрицей плотности при частичном транспонировании.
(ниже где-то он доказан)

Коррелированные (классическим и квантовым образом) состояния

Коррелированные состояния - это состояния, у которых $\rho_{AB} \neq \rho_A \otimes \rho_B$.
(?? только так определяются, никак иначе?)
Есть классическая корреляция, когда можно представить в виде выпуклой суммы

$$\rho_{AB} = \sum_k p_k \rho_A^k \otimes \rho_B^k$$

Есть квантовая корреляция, когда

$$\rho_{AB} \neq \sum_k p_k \rho_A^k \otimes \rho_B^k$$

это же запутанность.
Свойства:
множество всех сепарабельных состояний для данной системы выпукло.

Запутанные состояния

Запутанность, это когда

$$\rho_{AB} \neq \sum_k p_k \rho_A^k \otimes \rho_B^k$$

Критерии:
ранг Шмидта больше 2.
(по определению его, см. разложение Шмидта.)
(?? примеры !!!)
Свойства:
множество всех квантово перепутанных состояний для данной системы не выпукло.
(?? энтропия перепутанности???)
Также есть:
максимально перепутанное состояние:
(напишу потом)

Квантовый инструмент

POVM - мера, соответствующая измерению

POVM - это мера E, которая сопоставляется каждому исходу,
удовлетворяющая $E = E^+ \geq 0$, и вероятность каждого исхода вычисляется по

$$p(i) = \mathrm{tr}(\rho E_i)$$

Теорема Озавы (?? что-то говорит)

Взаимно несмещенный базис (??!!)

Квантовый канал

Квантовый канал - это линейное, вполне положительное отображение, сохраняющее след.

(тут пояснение про вполне положительность, что за определение)

2.7.3 Openness and Closeness of a Quantum System

(introduce this concept and write what exactly is meant by it)

2.7.4 Coordinate and Momentum Operators (!!!)

(напишу четко про это потом, важные операторы, много может быть путаницы)

Radial momentum operator and angular momentum operator

(это прекрасно написано у Сузуки.)

Radial momentum operator and angular momentum operator Masatsugu Sei Suzuki Department of Physics, SUNY at Binghamton (Date: February 03, 2015)

(потом выпишу, эту теорию здесь уже представляю)

p_x, p_y as a function of p_r and p_ϕ

$$x = r\cos\phi, \quad y = r\sin\phi.$$

Дифференцирование по x связано с r и ϕ через правило цепочки:

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \phi}{\partial x}\frac{\partial}{\partial \phi}.$$

Используем явные выражения для производных:

$$\frac{\partial r}{\partial x} = \cos\phi, \qquad \frac{\partial \phi}{\partial x} = -\frac{\sin\phi}{r}.$$

Подставляем это в правило цепочки:

$$\frac{\partial}{\partial x} = \cos\phi\frac{\partial}{\partial r} - \frac{\sin\phi}{r}\frac{\partial}{\partial \phi}.$$

Теперь оператор p_x принимает вид:

$$p_x = -i\hbar\left(\cos\phi\frac{\partial}{\partial r} - \frac{\sin\phi}{r}\frac{\partial}{\partial \phi}\right).$$

$$p_x = \cos\phi p_r - \frac{\sin\phi}{r}p_\phi.$$

The same for p_y:

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial \phi}{\partial y}\frac{\partial}{\partial \phi}.$$

Производные выражаются как:

$$\frac{\partial r}{\partial y} = \sin\phi, \quad \frac{\partial \phi}{\partial y} = \frac{\cos\phi}{r}.$$

Следовательно:

$$\frac{\partial}{\partial y} = \sin\phi \frac{\partial}{\partial r} + \frac{\cos\phi}{r}\frac{\partial}{\partial \phi}.$$

3. Оператор импульса:
Подставляем это в выражение для p_y:

$$p_y = -i\hbar\left(\sin\phi\frac{\partial}{\partial r} + \frac{\cos\phi}{r}\frac{\partial}{\partial\phi}\right).$$

4. Выражение через p_r и p_ϕ:
Подставляем определения радиального и углового операторов импульса - $p_r = -i\hbar\frac{\partial}{\partial r}$, - $p_\phi = -i\hbar\frac{\partial}{\partial\phi}$.
Получаем:

$$p_y = \sin\phi p_r + \frac{\cos\phi}{r}p_\phi.$$

2.7.5 Coordinate and Momentum Representations

(!!!!!!!!!!!!!! need to write this better!!!)

Теория импульсного представления по Тахтаджаяну

Начнем со случая одной степени свободы и рассмотрим две естественных реализации коммутационных соотношений Гейзенберга. Они определяются свойством, что один из самосопряженных операторов P и Q «диагонален» (т. е. является оператором умножения на функцию в соответствующем гильбертовом пространстве).

В координатном представлении $\mathscr{H} = L^2(\mathbb{R}, dq)$ - это L^2-пространство на конфигурационном пространстве $\mathbb{R}$с координатой q, являющемся лагранжевым подпространством пространства $\mathbb{R}^2$, определяемым уравнением $p = 0$. Положим

$$D(Q) = \left\{\varphi \in \mathscr{H} : \int\limits_{-\infty}^{\infty} q^2|\varphi(q)|^2 dq < \infty\right\}$$

и для $\varphi \in D(Q)$ определим оператор Q как «оператор умножения на q »:

$$(Q\varphi)(q) = q\varphi(q), q \in \mathbb{R}$$

оправдывая название «координатное представление». Оператор координаты Q очевидно самосопряжен, и его проекторная мера задается формулой

$$(\mathrm{P}(E)\varphi)(q) = \chi_E(q)\varphi(q)$$

где χ_E - характеристическая функция борелевского подмножества $E \subseteq \mathbb{R}$. Поэтому $\operatorname{supp} P = \mathbb{R}$ и $\sigma(Q) = \mathbb{R}$.

Напомним, что спектр самосопряженного оператора A абсолютно непрерывен, если для любого $\psi \in \mathscr{H}, \|\psi\| = 1$, вероятностная мера ν_ψ,

$$\nu_\psi(E) = (\mathrm{P}_A(E)\psi, \psi)\,, \quad E \in \mathscr{B}(\mathbb{R})$$

абсолютно непрерывна относительно меры Лебега на $\mathbb{R}$.

Лемма 2.2.

Оператор координаты Q имеет абсолютно непрерывный спектр $\mathbb{R}$, и любой ограниченный оператор B, коммутирующий cQ, является функцией от $Q, B = f(Q)cf \in L^\infty(\mathbb{R})$.

ДОКАЗАТЕЛЬСТВО.

Из (2.12) следует, что $\nu_\psi(E) = \int\limits_E |\psi(q)|^2 dq$, и это доказывает первое утверждение. Дальше, ограниченный оператор B в $\mathscr{H}$ коммутирует с Q, если и только если $B\mathrm{P}(E) = \mathrm{P}(E)B$ для всех $E \in \mathscr{B}(\mathbb{R})$, и, используя (2.12), мы получаем

$$B\left(\chi_E \varphi\right) = \chi_E B(\varphi)$$

Выбирая в (2.13) $E = E_1$ и $\varphi = \chi_{E_2}$, где E_1 и E_2 имеют конечную меру Лебега, получаем

$$B\left(\chi_{E_1} \cdot \chi_{E_2}\right) = B\left(\chi_{E_1 \cap E_2}\right) = \chi_{E_1} B\left(\chi_{E_2}\right) = \chi_{E_2} B\left(\chi_{E_1}\right),$$

так что, обозначая $f_E = B\left(\chi_E\right)$, мы получаем $\operatorname{supp} f_E \subseteq E$ и

$$f_{E_1}|_{E_1 \cap E_2} = f_{E_2}|_{E_1 \cap E_2}$$

для любых $E_1, E_2 \in \mathscr{B}(\mathbb{R})$ с конечной мерой Лебега. Таким образом, существует измеримая функция f на $\mathbb{R}$, такая, что $f|_E = f_E|_E$ для любого $E \in \mathscr{B}(\mathbb{R})$ с конечной мерой Лебега. Линейное подпространство, натянутое на все $\chi_E \in L^2(\mathbb{R})$, плотно в $L^2(\mathbb{R})$, а оператор B непрерывен, так что получаем

$$(B\varphi)(q) = f(q)\varphi(q) \quad \text{для любого } \varphi \in L^2(\mathbb{R}).$$

Поскольку B - ограниченный оператор, $f \in L^\infty(\mathbb{R})$ и $\|B\| = \|f\|_\infty$.

ЗАмечание. По теореме Шварца о ядре оператор B можно представить в виде интегрального оператора с обобщенным функциональным ядром $K\left(q, q'\right)$. Тогда из коммутативности $BQ = QB$ следует, что в смысле обобщенных функций

$$\left(q - q'\right) K\left(q, q'\right) = 0,$$

так что K «пропорционально» дельта-функции Дирака, т. е.

$$K\left(q, q'\right) = f(q)\delta\left(q - q'\right),$$

для некоторого $f \in L^\infty(\mathbb{R})$. Это рассуждение обычно приводят в учебниках физики.

ЗАМЕчАниЕ. У оператора Q нет собственных векторов - уравнение на собственные значения

$$Q\varphi = \lambda\varphi$$

не имеет решений в $L^2(\mathbb{R})$. Однако в смысле обобщенных функций это уравнение имеет для каждого $\lambda \in \mathbb{R}$ единственное (с точностью до постоянного множителя) решение $\varphi_\lambda(q) = \delta(q - \lambda)$, и эти «обобщенные собственные функции», называемые также собственными функциями непрерывного спектра, порождают ядро Шварца единичного оператора I в $L^2(\mathbb{R})$. Это отражает тот факт, что оператор Q диагонален в координатном представлении.

ЗАМЕЧАНИЕ. Нормировку собственных функций непрерывного спектра $\varphi_\lambda(q)$ можно также определить условием, что для любого $\lambda \in \mathbb{R}$ функция

удовлетворяет условию

$$\Phi_\lambda(q) = \int_{\lambda_0}^{\lambda} \varphi_\mu(q) d\mu, \quad \Phi_\lambda \in L^2(\mathbb{R})$$

$$\lim_{\Delta \to 0} \frac{1}{\Delta} \|\Phi_{\lambda+\Delta} - \Phi_\lambda\|^2 = 1.$$

Здесь $\lambda_0 \in \mathbb{R}$ фиксировано и не входит в (2.14). Действительно, в нашем случае $\Phi_\lambda = \chi_{(\lambda_0,\lambda)}$ - характеристическая функция интервала (λ_0, λ), так что $\|\Phi_{\lambda+\Delta} - \Phi_\lambda\|^2 = \Delta$. Для чистого состояния $M = P_\psi, \|\psi\| = 1$ соответствующая вероятностная мера μ_Q на $\mathbb{R}$ дается формулой

$$\mu_Q(E) = \nu_\psi(E) = \int_E |\psi(q)|^2 dq, \quad E \in \mathscr{B}(\mathbb{R}).$$

Физически это интерпретируется так, что в состоянии P_ψ с «волновой функцией» $\psi(q)$ вероятность нахождения квантовой частицы между q и $q + dq$ равна $|\psi(q)|^2 dq$. Другими словами, квадрат модуля волновой функции - это распределение вероятности координаты квантовой частицы.

Соответствующий оператор импульса P дается дифференциальным оператором

$$P = \frac{\hbar}{i} \frac{d}{dq}$$

с $D(P) = W^{1,2}(\mathbb{R})$ - пространством Соболева абсолютно непрерывных функций f на $\mathbb{R}$, таких, что f и ее производная f' (определенная п. в.) принадлежат $L^2(\mathbb{R})$. Оператор P самосопряжен, и не составляет труда проверить, что на $D = C_c^\infty(\mathbb{R})$, пространстве гладких функций на $\mathbb{R}$ с компактным носителем,

$$QP - PQ = i\hbar I.$$

Замечание. У оператора P в $\mathscr{H}$ нет собственных векторов, уравнение на собственные значения

$$P\varphi = p\varphi, p \in \mathbb{R}$$

имеет решение

$$\varphi(q) = \text{ const } \times e^{\frac{i}{\hbar} pq}$$

не принадлежащее $L^2(\mathbb{R})$. Мы увидим впоследствии, что семейство нормированных собственных функций непрерывного спектра

$$\varphi_p(q) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} pq}$$

порождает ядро Шварца обратного к зависящему от $\hbar$ преобразованию Фурье оператора, диагонализующего оператор импульса P. В смысле обобщенных функций

$$\int_{-\infty}^{\infty} \varphi_p(q) \overline{\varphi_{p'}(q)} dq = \delta(p - p').$$

ЗАМЕчАНиЕ. Как и в случае оператора координаты, нормировку собственных функций непрерывного спектра $\varphi_p(q)$ оператора импульса можно определить условием (2.14). Действительно,

$$\Phi_p(q) = \int_{p_0}^{p} ce^{\frac{i}{\hbar}kq}dk = \frac{c\hbar}{iq}\left(e^{\frac{i}{\hbar}pq} - e^{\frac{i}{\hbar}p_0q}\right)$$

так что

$$\Phi_{p+\Delta}(q) - \Phi_p(q) = \frac{2c\hbar}{q}e^{\frac{i}{\hbar}\left(p+\frac{1}{2}\Delta\right)q}\sin\frac{\Delta q}{2\hbar}$$

Используя элементарное интегрирование, получаем

$$\frac{1}{\Delta}\left\|\Phi_{p+\Delta}(q) - \Phi_p(q)\right\|^2 = 2c^2\hbar\int_{-\infty}^{\infty}\frac{\sin^2 q}{q^2}dq = 2\pi c^2\hbar$$

так что $c = \frac{1}{\sqrt{2\pi\hbar}}$.

Предложение 2.1.

Координатное представление определяет неприводимое, унитарное, интегрируемое представление алгебры Гейзенберга.

ДокАЗАтЕЛЬство.

Чтобы показать, что координатное представление интегрируемо, положим $U(u) = e^{-iuP}$, и пусть $V(v) = e^{-ivQ}$ - соответствующая однопараметрическая группа унитарных операторов. Ясно, что $(V(v)\varphi)\psi(q) = e^{-ivq}\varphi(q)$, и из теоремы Стоуна (или из определения производной) легко выводится, что $(U(u)\varphi)(q) = \varphi(q - \hbar u)$, так что унитарные операторы $U(u)$ и $V(v)$ удовлетворяют соотношению Вейля (2.11). Такая реализация соотношения Вейля называется представлением Шрёдингера.

Для доказательства неприводимости координатного представления выберем ограниченный оператор T, коммутирующий с P и Q. По лемме 2.2$T = f(Q)$ для какого-то $f \in L^\infty(\mathbb{R})$. Дальше, из коммутативности T и P следует, что

$$TU(u) = U(u)T \quad \text{для любого} \quad u \in \mathbb{R}$$

а это эквивалентно тому, что $f(q - \hbar u) = f(q)$ для любых $q, u \in \mathbb{R}$, так что $f = \text{const}$ п. в. на $\mathbb{R}$.

В итоге координатное представление характеризуется свойством, что оператор координаты Q - это умножение на q, а оператор импульса P - это дифференцирование:

$$Q = q \quad \text{и} \quad P = \frac{\hbar}{i}\frac{d}{dq}$$

Аналогично, импульсное представление определяется свойством, что оператор импульса P - это умножение на p. А именно: пусть $\mathscr{H} = L^2(\mathbb{R}, dp)$ - гильбертово L^2-пространство на «пространстве импульсов» $\mathbb{R}$ с координатой p, являющемся лагранжевым подпространством в $\mathbb{R}^2$, определенным уравнением $q = 0$. Операторы координаты и импульса даются формулами

$$\hat{Q} = i\hbar\frac{d}{dp} \quad \text{и} \quad \hat{P} = p$$

и удовлетворяют коммутационному соотношению Гейзенберга. Как и координатное представление, импульсное представление - неприводимое, унитарное, интегрируемое представление алгебры Гейзенберга. В импульсном представлении квадрат модуля волновой функции $\psi(p)$ чистого состояния $M = P_\psi, \|\psi\| = 1$, есть распределение вероятности импульса квантовой частицы, т. е. вероятность, что квантовая частица имеет импульс, заключенный между p и $p + dp$, равна $|\psi(p)|^2 dp$.

Пусть $\mathscr{F}_\hbar : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ - оператор зависящего от $\hbar$ преобразования Фурье, определенный формулой

$$\hat{\varphi}(p) = \mathscr{F}_\hbar(\varphi)(p) = \frac{1}{\sqrt{2\pi\hbar}} \int\limits_{-\infty}^{\infty} e^{-\frac{i}{\hbar}pq} \varphi(q) dq$$

Здесь интеграл понимается как предел $\hat{\varphi} = \lim_{n\to\infty} \hat{\varphi}_n$ в сильной топологии $L^2(\mathbb{R})$, где

$$\hat{\varphi}_n(p) = \frac{1}{\sqrt{2\pi\hbar}} \int\limits_{-n}^{n} e^{-\frac{i}{\hbar}pq} \varphi(q) dq$$

По теореме Планшереля $\mathscr{F}_\hbar$ - унитарный оператор в $L^2(\mathbb{R})$,

$$\mathscr{F}_\hbar \mathscr{F}_\hbar^* = \mathscr{F}_\hbar^* \mathscr{F}_\hbar = I,$$

K

$$\hat{Q} = \mathscr{F}_\hbar Q \mathscr{F}_\hbar^{-1}, \quad \hat{P} = \mathscr{F}_\hbar P \mathscr{F}_\hbar^{-1},$$

так что координатное и импульсное представления унитарно эквивалентны. В частности, поскольку оператор $\hat{P}$ очевидно самосопряжен, это мгновенно показывает, что и оператор P самосопряжен.

Для n степеней свободы координатное представление определяется заданием $\mathscr{H} = L^2\left(\mathbb{R}^n, d^n\boldsymbol{q}\right)$, где $d^n\boldsymbol{q} = dq^1 \cdots dq^n$ - мера Лебега на $\mathbb{R}^n$, и

$$\boldsymbol{Q} = \boldsymbol{q} = \left(q^1, ..., q^n\right), \quad \boldsymbol{P} = \frac{\hbar}{i}\frac{\partial}{\partial \boldsymbol{q}} = \left(\frac{\hbar}{i}\frac{\partial}{\partial q^1}, ..., \frac{\hbar}{i}\frac{\partial}{\partial q^n}\right).$$

Здесь $\mathbb{R}^n$ - конфигурационное пространство с координатами $\boldsymbol{q}$ - лагранжево подпространство $\mathbb{R}^{2n}$, определяемое уравнениями $\boldsymbol{p} = 0$. Операторы координат и импульсов самосопряжены и удовлетворяют коммутационным соотношениям Гейзенберга. Проекторные меры операторов Q^k даются формулами

$$\left(\mathrm{P}_k(E)\varphi\right)(\boldsymbol{q}) = \chi_{\lambda_k^{-1}(E)}(\boldsymbol{q})\varphi(\boldsymbol{q}),$$

где $E \in \mathscr{B}(\mathbb{R})$, а $\lambda_k : \mathbb{R}^n \to \mathbb{R}$ - каноническая проекция на k-ю компоненту, $k = 1, ..., n$. Соответственно, проекторная мера P коммутативного семейства $\boldsymbol{Q} = (Q^1, ..., Q^n)$ (см. предложение 1.3) определяется на борелевских подмножествах $\boldsymbol{E} \subseteq \mathbb{R}^n$ формулой

$$(\mathrm{P}(\boldsymbol{E})\varphi)(\boldsymbol{q}) = \chi_{\boldsymbol{E}}(\boldsymbol{q})\varphi(\boldsymbol{q}).$$

Семейство $\boldsymbol{Q}$ имеет абсолютно непрерывный совместный спектр $\mathbb{R}^n$.

Координатные операторы $Q^1, ..., Q^n$ образуют полную систему коммутирующих наблюдаемых. Это по определению означает, что ни один из этих операторов не является функцией оставшихся, и что любой ограниченный оператор, коммутирующий с $Q^1, ..., Q^n$, - функция $Q^1, ..., Q^n$, т. е. оператор умножения на $f(\boldsymbol{q})$ для какого-то $f \in L^\infty\left(\mathbb{R}^n\right)$. Доказательство дословно повторяет доказательство леммы 2.2. Для чистого состояния

$M = P_\psi, \|\psi\| = 1$, квадрат модуля $|\psi(\boldsymbol{q})|^2$ волновой функции - это плотность совместной функции распределения $\mu_{\boldsymbol{Q}}$ коммутативного семейства $\boldsymbol{Q}$, т. е. вероятность нахождения квантовой частицы в борелевском подмножестве $\boldsymbol{E} \subseteq \mathbb{R}^n$ дается формулой

$$\mu_{\boldsymbol{Q}}(\boldsymbol{E}) = \int\limits_{\boldsymbol{E}} |\psi(\boldsymbol{q})|^2 d^n\boldsymbol{q}$$

Координатное представление определяет неприводимое, унитарное, интегрируемое представление алгебры Гейзенберга $\mathfrak{h}_n$. Действительно, n параметрические группы унитарных операторов $U(\boldsymbol{u}) = e^{-i\boldsymbol{u}\boldsymbol{P}}$ и $V(\boldsymbol{v}) = e^{-iv\boldsymbol{Q}}$ описываются формулами

$$(U(\boldsymbol{u})\varphi)(\boldsymbol{q}) = \varphi(\boldsymbol{q} - \hbar\boldsymbol{u}), \quad (V(\boldsymbol{v})\varphi)(\boldsymbol{q}) = e^{-i\boldsymbol{v}\boldsymbol{q}}\varphi(\boldsymbol{q})$$

и удовлетворяют соотношениям Вейля (2.11). То же рассуждение, что и в доказательстве предложения 2.1 показывает, что это представление группы Гейзенберга $\mathbf{H}_n$, называемое представлением Шрёдингера для n степеней свободы, неприводимо. В импульсном представлении $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{p})$, где $d^n\boldsymbol{p} = dp_1 \cdots dp_n$ - мера Лебега на $\mathbb{R}^n$, и

$$\hat{\boldsymbol{Q}} = i\hbar\frac{\partial}{\partial \boldsymbol{p}} = \left(i\hbar\frac{\partial}{\partial p_1}, ..., i\hbar\frac{\partial}{\partial p_n}\right), \quad \hat{\boldsymbol{P}} = \boldsymbol{p} = (p_1, ..., p_n).$$

Здесь $\mathbb{R}^n$ - это пространство импульсов с координатами $\boldsymbol{p}$ - лагранжево подпространство $\mathbb{R}^{2n}$, определенное уравнениями $\boldsymbol{q} = 0$.

Координатное и импульсное представления унитарно эквивалентны через преобразование Фурье. Как и в случае $n = 1$, преобразование Фурье $\mathscr{F}_\hbar : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ - это унитарный оператор, определенный формулой

$$\hat{\varphi}(\boldsymbol{p}) = \mathscr{F}_\hbar(\varphi)(\boldsymbol{p}) = (2\pi\hbar)^{-n/2} \int\limits_{\mathbb{R}^n} e^{-\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{q}}\varphi(\boldsymbol{q})d^n\boldsymbol{q} =$$

$$= \lim_{N\to\infty} (2\pi\hbar)^{-n/2} \int\limits_{|\boldsymbol{q}|\leqslant N} e^{-\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{q}}\varphi(\boldsymbol{q})d^n\boldsymbol{q},$$

где предел понимается в сильной топологии на $L^2(\mathbb{R}^n)$. Как в случае $n = 1$, имеем

$$\hat{Q}_k = \mathscr{F}_\hbar Q_k \mathscr{F}_\hbar^{-1}, \quad \hat{P}_k = \mathscr{F}_\hbar P_k \mathscr{F}_\hbar^{-1}, \quad k = 1, ..., n.$$

В частности, поскольку операторы $\hat{P}_1, ..., \hat{P}_n$, очевидно, самосопряжены, это мгновенно показывает, что $P_1, ..., P_n$ тоже самосопряжены.

ЗАМЕчАНиЕ. Следуя Дираку, физики обозначают вектор $\psi \in \mathscr{H}$ кетвектором $|\psi\rangle$, вектор $\varphi \in \mathscr{H}^*$ в двойственном к $\mathscr{H}$ пространстве ($\mathscr{H}^* \simeq \mathscr{H}$ - комплексный антилинейный изоморфизм) - бра-вектором $\langle\varphi|$, а их скалярное произведение - выражением $\langle\varphi|\psi\rangle$. В стандартных математических обозначениях

$$(\psi, \varphi) = \langle\varphi|\psi\rangle \quad \text{и} \quad (A\psi, \varphi) = \langle\varphi|A|\psi\rangle,$$

где A - линейный оператор. С физической точки зрения дираковские обозначения соответствуют интуиции и удобны для работы с координатным и импульсным представлениями. Обозначив как $|\boldsymbol{q}\rangle = \delta(\boldsymbol{q} - \boldsymbol{q}')$ и $|\boldsymbol{p}\rangle = (2\pi\hbar)^{-n/2}e^{\frac{i}{\hbar}pq}$ множества общих обобщенных собственных функций операторов $\boldsymbol{Q}$ и $\boldsymbol{P}$ соответственно; мы формально получаем

$$\boldsymbol{Q}|\boldsymbol{q}\rangle = \boldsymbol{q}|\boldsymbol{q}\rangle, \quad \boldsymbol{P}|\boldsymbol{p}\rangle = \boldsymbol{p}|\boldsymbol{p}\rangle$$

где операторы $\mathbf{Q}$ действуют на $\boldsymbol{q}'$, и

$$\langle \boldsymbol{q}|\psi\rangle = \int\limits_{\mathbb{R}^n} \delta\left(\boldsymbol{q}-\boldsymbol{q}'\right)\psi\left(\boldsymbol{q}'\right)d^n\boldsymbol{q}' = \psi(\boldsymbol{q}),$$

$$\langle \boldsymbol{p}|\psi\rangle = (2\pi\hbar)^{-n/2}\int\limits_{\mathbb{R}^n} e^{-\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{q}}\psi(\boldsymbol{q})d^n\boldsymbol{q} = \hat{\psi}(\boldsymbol{p}),$$

так же как $\langle \boldsymbol{q}|\boldsymbol{q}'\rangle = \delta\left(\boldsymbol{q}-\boldsymbol{q}'\right), \langle \boldsymbol{p}|\boldsymbol{p}'\rangle = \delta\left(\boldsymbol{p}-\boldsymbol{p}'\right)$. Хотя в нашем изложении мы не используем дираковские обозначения, эти формулы могут помочь заинтересованному читателю «переводить» обозначения из учебников физики на стандартный математический язык.

ЗАМЕчАниЕ. Мы покажем в разделе 2.3.2, что любое лагранжево подпространство симплектического векторного пространства $\mathbb{R}^{2n}$ с канонической симплектической формой $\omega = dp \wedge d\boldsymbol{q}$ порождает интегрируемое, унитарное, неприводимое представление алгебры Гейзенберга $\mathfrak{h}_n$. Это простейший пример действительной поляризачии, определяемой для заданного симплектического многообразия $(\mathscr{M}, \omega)$ как интегрируемое распределение $\{\mathscr{L}_x\}_{x\in\mathscr{M}}$ лагранжевых подпространств $\mathscr{L}_x$ касательных пространств $T_x\mathscr{M}$. Понятие поляризации играет фундаментальную роль в геометрическом квантовании: оно позволяет построить (при определенных условиях) гильбертово пространство состояний $\mathscr{H}$, ассоциированное с классическим фазовым пространством $(\mathscr{M}, \omega)$. В линейном случае $\mathscr{M} = \mathbb{R}^{2n}$, любое лагранжево подпространство $\mathscr{L}$ в $\mathbb{R}^{2n}$ порождает действительную поляризацию через идентификацию $T_x\mathbb{R}^{2n} \simeq \mathbb{R}^{2n}$. В частности, для координатного представления $\mathscr{L}$ дается уравнением $\boldsymbol{q} = 0$, а для импульсного - уравнением $\boldsymbol{p} = 0$. Соответствующее гильбертово пространство $\mathscr{H}$ состоит из функций на $\mathbb{R}^{2n}$, постоянных на слоях поляризации.

ЗАДАчА 2.4. Приведите пример неинтегрируемого представления алгебры Гейзенберга.

ЗАДАЧА 2.5. Докажите, что существует $\varphi \in \mathscr{H} = L^2(\mathbb{R}, dq)$, такое, что векторы $\mathrm{P}(E)\varphi, E \in \mathscr{B}(\mathbb{R})$, где P - проекторная мера оператора координаты Q, плотны в $\mathscr{H}$.

ЗАДАЧА 2.6. Найдите порождающий оператор для коммутативного семейства $\boldsymbol{Q} = (Q^1, ..., Q^n)$. Есть ли у него физическая интерпретация?

ЗАДАЧА 2.7. Найдите проекторную меру коммутативного семейства $\boldsymbol{P} = (P_1, ..., P_n)$ в координатном представлении.

Interaction in coordinate and momenta representation

(??? how exactly this happens??)

Meaning of second quantization in coordinate and momenta representation

(??? that Fourier transform, what is this meaning??)
(??? how exactly this happens??)

Does a number of particle makes sense from the point of view of existence of coordinate and momenta representation

(??? the question about that Fourier transform makes from one function sum of a lot of functions, maybe 100 functions. so how many particles are there? or only coordinate representation is physical?)

Is momentum representation really useful?

(discuss this!!! I don't know, I am not convinced.)
(what if there was no momenta repr in general?)
(what if there was no momenta repr in scatteing theory?)
(what if there was no momenta repr in cond matter systems?)

2.7.6 De Broglie Waves and the Connection of QM with Optics (????)

Суть

Понятие луча (??)

Какое соотношение эквивалентности задает понятие луча в пространстве квантовых состояний физической системы?
(Вопросы Киселева на развлечение (?!!!!!))

Спиноры ведь строго говоря представляют из себя более сложную волну, чем обычная волна? (?????)

Пока не знаю. Получается, вообще неверная формула для волны де бройля, потому что она не учитывает спин.

Как учесть спин частицы в волне де Бройля? (?????)

(?????? не знаю, два формлизма еще не усвоил, когда-то отвечу на этот вопрос, пока качество записи не такое еще.)

Другое

До какой скорости нужно разогнать человека, чтобы он проявил волновые свойства? (????)

(пока не знаю.)

2.7.7 Wave Packet (???)

Обсудим подробно волновой пакет

Расплывание волнового пакета (!??!)

(типичный вопрос, что с этим делать (!??!?) пока так и не понял.)

Не стоит ли вообще забить на квантовую механику из-за этого???

Или такая природа, что все и должно расплываться??? хз.

движение максимума фазы

Посмотрим, как движется максимум фазы.

Условие максимума имеет вид: $\frac{\partial \phi}{\partial p} = 0$, тогда расписывая с учетом уравнения движения:

$$r - \frac{\partial E}{\partial \boldsymbol{p}} t + \hbar \frac{\partial \alpha}{\partial p} = 0$$

И вводится групповая скорость:

$$\boldsymbol{v}_{\text{gr}} = \frac{\partial E}{\partial \boldsymbol{p}}$$

2.7.8 Concept of Quantum Field

(I'll describe in details, what is it. general intro to qft)

2.7.9 Superposition Principle (??)

Обсудим подробно принцип суперпозиции.

2.7.10 Probability Current

(тоже про него тут всё)

2.7.11 Concept of Density Matrix 1: Basics

Приведем общие соображения про матрицу плотности и ее появление.

Density matrix by Nielsen, Chang

(write his version)

Density matrix by Tokmakoff

The density matrix or density operator is an alternate representation of the state of a quantum system for which we have previously used the wavefunction. Although describing a quantum system with the density matrix is equivalent to using the wavefunction, one gains significant practical advantages using the density matrix for certain time-dependent problemsparticularly relaxation and nonlinear spectroscopy in the condensed phase.

The density matrix is defined as the outer product of the wavefunction with its conjugate.

$$\rho(t) \equiv |\psi(t)\rangle\langle\psi(t)|$$

This implies that if you specify a state $|x\rangle$, then $\langle x|\rho|x\rangle$ gives the probability of finding a particle in the state $|x\rangle$. Its name derives from the observation that it plays the quantum role of a probability density. If you think of the statistical description of a classical observable obtained from moments of a probability distribution P, then ρ plays the role of P in the quantum case:

$$\begin{aligned}\langle A\rangle &= \int AP(A)dA \\ &= \langle\psi|A|\psi\rangle = \text{Tr}[A\rho]\end{aligned}$$

where Tr[...] refers to tracing over the diagonal elements of the matrix,

$$\mathrm{Tr}[\cdots] = \sum_a \langle a| \cdots |a\rangle$$

The last expression is obtained as follows. If the wavefunction for the system is expanded as

$$|\psi(t)\rangle = \sum_n c_n(t)|n\rangle$$

the expectation value of an operator is

$$\langle \hat{A}(t)\rangle = \sum_{n,m} c_n(t)c_m^*(t)\langle m|\hat{A}|n\rangle$$

Also, from Equation 5.1.1 we obtain the elements of the density matrix as

$$\begin{aligned}\rho(t) &= \sum_{n,m} c_n(t)c_m^*(t)|n\rangle\langle m| \\ &\equiv \sum_{n,m} \rho_{nm}(t)|n\rangle\langle m|\end{aligned}$$

We see that ρ_{nm}, the density matrix elements, are made up of the time-evolving expansion coefficients. Substituting into Equation 5.1.6 we see that

$$\begin{aligned}\langle \hat{A}(t)\rangle &= \sum_{n,m} A_{mn}\rho_{nm}(t) \\ &= \mathrm{Tr}[\hat{A}\rho(t)]\end{aligned}$$

In practice this makes evaluating expectation values as simple as tracing over a product of matrices. What information is in the density matrix elements, ρ_{nm} ? The diagonal elements $(n = m)$ give the probability of occupying a quantum state:

$$\rho_{nn} = c_n c_n^* = p_n \geq 0$$

For this reason, diagonal elements are referred to as populations. The off-diagonal elements ($n \neq m$) are complex and have a time-dependent phase factor

$$\rho_{nm} = c_n(t)c_m^*(t) = c_n c_m^* \mathrm{e}^{-i\omega_{nm}t}$$

Since these describe the coherent oscillatory behavior of coherent superpositions in the system, these are referred to as coherences.

So why would we need the density matrix? It becomes a particularly important tool when dealing with mixed states, which we take up later. Mixed states refer to statistical mixtures in which we have imperfect information about the system, for which me must perform statistical averages in order to describe quantum observables. For mixed states, calculations with the density matrix are greatly simplified. Given that you have a statistical mixture, and can

describe p_k, the probability of occupying quantum state $|\psi_k\rangle$, evaluation of expectation values is simplified with a density matrix:

$$\langle \hat{A}(t) \rangle = \sum_k p_k \langle \psi_k(t) | \hat{A} | \psi_k(t) \rangle$$
$$\rho(t) \equiv \sum_k p_k |\psi_k(t)\rangle \langle \psi_k(t)|$$
$$\langle \hat{A}(t) \rangle = \mathrm{Tr}[\hat{A}\rho(t)]$$

Evaluating expectation value is the same for pure or mixed states.

Density matrix: Other questions

(overview of many other related things to this concept)

явный пример выделения из одной системы двух подсистем

Об уравнениях открытых систем

про Линдблада чуть скажу.
мб про другие уравнения

Examples of density matrices

(just to clarify the concept)

примеры открытых систем

Пример, когда волновой функции не достаточно

(четко этот пример укажу, пока что хз)

General conceptual questions about density matrix

связь с другими описаниями

с волновой функцией?
с обычной функцией распределения???
очень актуально!

О случаях применения матрицы плотности и открытых систем (?!!)

(очень важно прописать нормально, когда они нужны!!?? пока не особо применял.)
- в квантовой теории информации
(тут большое описание, насколько она важна там! достаточно в принципе важна)

Динамика систем, описываемых матрицей плотности

Динамика матрицы плотности описывается с помощью уравнения Гейзенберга:

$$\frac{\partial \hat{\rho}}{\partial t} = \frac{i}{\hbar}[\hat{\rho}(t), \hat{H}]$$

Чтобы это увидеть, нужно просто взять производную по времени от матрицы плотности: $\hat{\rho}(t) = \sum_{mn}\langle n(t)|\rho_{nm}|m(t)\rangle$. Добавка в уравнение полученное тождество уравнения Шредингера завершит доказательство:

$$i\hbar\frac{\partial\hat{\rho}}{\partial t} = \sum_{mn}\left[i\hbar\frac{\partial|n(t)\rangle}{\partial t}\rho_{nm}\langle m(t)| + i\hbar|n(t)\rangle\rho_{nm}\frac{\partial\langle m(t)|}{\partial t}\right] =$$
$$= \sum_{mn}\left[\hat{H}|n(t)\rangle\rho_{nm}\langle m(t)| - |n(t)\rangle\rho_{nm}\langle m(t)|\hat{H}\right] = [\hat{H},\hat{\rho}(t)]$$

(тут еще много про динамику можно будет добавить)

Динамика систем, описываемых матрицей плотности: Conceptual questions

основы термодинамики открытых квантовых систем

(тут общие рассуждения)
Таким образом,

$$\hat{\rho} = \frac{1}{Z}e^{-\beta\hat{H}},$$

где $Z = \mathrm{Tr}\left(e^{-\beta\hat{H}}\right) = \sum_n e^{-\beta E_n}$

(и что?)

Пример взаимодействие среды с окружением

пример: взаимодействие среды с окружением
(говорят, она для этого нужна)

Пример разделение систем на подсистемы и состояния

разделение систем на подсистемы и состояния
в простом случае, если системы разделяются, то $\rho(x,x') = \Psi(x)\Psi*(x')$ и такое состояние называется *чистым* .
что мы всегда при измеренеии можем получать смешанные состояния - супперпозицию чистых.
(?)
тема очень важная, тут как раз ответим про состояние на все вопросы.
по сути мы уже многим владеем и все можем сказать.
теперь поговорим про ЭПР
У морозова есть методичка про это, до которой скорее всего я не дойду, но она гуглится.

обзор применений открытых систем

что с ними можно описать?

2.7.12 Concept of Density Matrix 1: Other Approaches

Density matrix by Landau

(write his version)

Density matrix by Brewer Petrucione

(write their version, see note on kinetics for now)

The Density Matrix in the Interaction Picture by Tokmakoff

For the case in which we wish to describe a material Hamiltonian H_0 under the influence of an external potential $V(t)$,

$$H(t) = H_0 + V(t)$$

we can also formulate the density operator in the interaction picture, ρ_I. From our original definition of the interaction picture wavefunctions

$$|\psi_I\rangle = U_0^\dagger |\psi_S\rangle$$

We obtain ρ_I as

$$\rho_I = U_0^\dagger \rho_S U_0$$

Similar to the discussion of the density operator in the Schrödinger equation, above, the equation of motion in the interaction picture is

$$\frac{\partial \rho_I}{\partial t} = -\frac{i}{\hbar}\left[V_I(t), \rho_I(t)\right]$$

where, as before, $V_I = U_0^\dagger V U_0$. Equation 5.3.4 can be integrated to obtain

$$\rho_I(t) = \rho_I\left(t_0\right) - \frac{i}{\hbar}\int_{t_0}^{t} dt' \left[V_I\left(t'\right), \rho_I\left(t'\right)\right]$$

Repeated substitution of $\rho_I(t)$ into itself in this expression gives a perturbation series expansion

$$\begin{aligned}
\rho_I(t) &= \rho_0 - \frac{i}{\hbar}\int_{t_0}^{t} dt_2 \left[V_I\left(t_1\right), \rho_0\right] \\
&+ \left(-\frac{i}{\hbar}\right)\int_{t_0}^{t} dt_2 \int_{t_0}^{t_2} dt_1 \left[V_I\left(t_2\right), \left[V_I\left(t_1\right), \rho_0\right]\right] + \cdots \\
&+ \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_n \int_{t_0}^{t_n} dt_{n-1} \cdots \int_{t_0}^{t_2} dt_1 \left[V_I\left(t_n\right), \left[V_I\left(t_{n-1}\right), \cdots \left[V_I\left(t_1\right), \rho_0\right]\right]\right] \\
&= \rho^{(0)} + \rho^{(1)} + \rho^{(2)} + \cdots + \rho^{(n)} + \cdots
\end{aligned}$$

Here $\rho_0 = \rho\left(t_0\right)$ and $\rho^{(n)}$ is the n^{th} -order expansion of the density matrix. This perturbative expansion will play an important role later in the description of nonlinear spectroscopy. An n^{th} order expansion term will be proportional to the observed polarization in an n^{th} -order nonlinear spectroscopy, and the commutators observed in Equation 5.3.8 are closely related to nonlinear response functions. Equation 5.3.8 can also be expressed as

$$\rho_I(t) = U_0 \rho_I(0) U_0^\dagger$$

This is the solution to the Liouville equation in the interaction picture.

2.7.13 How to Use QM for Many-Particle Systems?

(general intro to cond matter. like, okay, we know that there is a wave function, that we also can introduce creation operators, so how to describe a conductor? this is also written in the note on cond matter. I want to make this connection more explicit.)

2.8 Other, Useful Operators

(here, there are operators, which will be used, but they don't really need a special section, this section here is just for completeness, since for one it can be comfortable to have a collection of their properties in one place)

2.8.1 Form of a Spectrum of a Particle

(connect it with Noether's theorem, why it can be? seriously! why in cond matter there are different spectrums?)

2.8.2 Evolution Operator

Обсудим подробно оператор эволюции.

Типичные свойства

Согласно современному пониманию квантовой механики, любые материальные объекты состоят из частиц, которые могут быть в различных состояниях.

Состояние частицы полностью определяется амплитудой вероятности $\Psi(q)$ того, что частица имеет определенные точные значения своих наблюдаемых $\{q\}$.

Амплитуда вероятности определяет волновую сущность состояния частицы, потому также называется волновой функцией.

Переход от амплитуды вероятности к вероятности происходит просто: $w = |\psi(q)|^2$.

Поэтому суммарная вероятность всех состояний должна быть 1:

$$\sum_{\{q\}} |\psi(q, t_0)|^2 = 1$$

Есть и другие очевидные свойства волновой функции, такие как непрерывность (но не гладкости требовать не нужно), интегрируемость,

Динамика волновой функции определяется оператором эволюции $\hat{U}(t)$

$$|\Psi(t)\rangle = \hat{U}(t)|\Psi\rangle$$

При этом должна сохраняться нормировка:

$$\langle\Psi(t)|\Psi(t)\rangle = 1$$

А так как можно переходить к эрмитово сопряженному оператору как $\left\langle A^\dagger\Psi|\Phi\right\rangle = \langle\Psi|A\Phi\rangle$, то

$$\begin{aligned}\langle\Psi(t)|\Psi(t)\rangle = \langle U(t)\Psi|U(t)\Psi\rangle &= \left\langle U^\dagger(t)U(t)\Psi|\Psi\right\rangle \\ \left\langle U^\dagger(t)U(t)\Psi|\Psi\right\rangle &= \langle\Psi|\Psi\rangle \quad \leftrightarrow \quad \hat{U}^\dagger\hat{U} = \hat{1}\end{aligned}$$

Это свойство оператора эволюции называется унитарностью.

Волновая функция состояния системы эволюционирует согласно уравнению Шредингера

$$i\hbar\frac{\partial|\Psi\rangle}{\partial t} = \hat{H}|\Psi\rangle,$$

здесь $\hat{H}$ - гамильтониан, соответствующий данной системе.

Его связь с оператором эволюции легко получить, подставив в уравнение Шредингера этот оператор, и в случае гамильтониана, не зависящего от времени, имеет вид:

$$i\hbar\frac{\partial\hat{U}(t)}{\partial t} = \hat{H}\hat{U}(t) \quad \rightarrow \quad \hat{U}(t) \equiv \exp(-i\hat{H}t/\hbar)$$

Преобразования при замене базиса

При замене базиса унитарными преобразованиями $|\psi'\rangle = \hat{U}|\psi\rangle$.

1. Покажите, что гамильтониан при этом заменяется на $\hat{H}' = \hat{U}\hat{H}\hat{U}^\dagger$.

2. Последнее утверждение необходимо модифицировать, если унитарное преобразование зависит явно от времени $\hat{U} = \hat{U}(t)$. Покажите, что в таком случае гамильтониан необходимо заменить на $\hat{H}' = \hat{U}\hat{H}\hat{U}^\dagger - i\hbar\hat{U}\partial_t\hat{U}^\dagger$.

(простое свойство, потом раскрою, ничего такого нет в этом.)

Другие свойства оператора эволюции (??)

(тут многое потом связано с ним, у Киселева спишу)

Как догадаться про оператор эволюции?

2.8.3 Particle Number Operator

Обсудим подробно оператор числа частиц.

2.9 Concept of Measurement in QM

(see note on quantum information for details)

2.9.1 Measurement Method

(тут подробно отвечаю про это. мб в часть про строгий квантмех тоже добавлю, в то же время в 1й части параграф будет с сутью этого)

измерения как особенное сопоставление борелевских мер алгебре наблюдаемых

там всякое задротство
определять алгебру наблюдаемых

Парадокс Эйнштейна-Подольского-Розена

(птф 2 лекция + методичка морозова тут)

$$\hat{\rho}_{AB} = |\psi_{AB}\rangle\langle\psi_{AB}| = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\hat{\rho}_A = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}\hat{\mathbb{I}}$$

сравним с классической: носки

$$\hat{\rho}_{AB} = \frac{1}{2}\left(\hat{\mathbb{P}}_{\uparrow\downarrow} + \hat{\mathbb{P}}_{\downarrow\uparrow}\right) = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\hat{\rho}_A = \mathrm{Tr}_B\, \hat{\rho}_{AB} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}\hat{\mathbb{I}}$$

Редукция фон неймана в двух словах (???)

(потом напишу)

????? Зачастую когда речь заходит об измерениях, используется механизм Фон Неймана, так что обсудим его тут.

??? после измерения $\hat{\rho}_m$????

измерение происходит по формуле??

$$\hat{\rho}_m \sum_n \mathbb{P}_n \hat{\rho} \hat{\mathbb{P}}_n \leftrightarrow \begin{pmatrix} \rho_{11} & \rho_{12} & \dots & \rho_{1n} \\ \rho_{21} & \rho_{22} & \dots & \rho_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{n1} & \rho_{n2} & \dots & \rho_{nn} \end{pmatrix} \mapsto \begin{pmatrix} \rho_{11} & 0 & \dots & 0 \\ 0 & \rho_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \rho_{nn} \end{pmatrix}$$

Такое изменение матрицы плотности является объективным результатом взаимодействия системы с измеряющим прибором.

Во-первых, мы ничего не говорили о результате измерений, узнали ли мы его или нет.

Во-вторых, оно затронет результаты последующих измерений любой другой наблюдаемой, в базисе которой матрица плотности недиагональна (т.е. которая не коммутирует с O), поэтому это — наблюдаемый эффект.

Наконец, на некоторых конкретных моделях можно аккуратно проследить, как такая диагонализация происходит в результате унитарной эволюции — взаимодействия с окружающей средой.

«Вымирание» оффдиагональных элементов матрицы плотности в результате взаимодействия с окружающей средой носит название дефазировки или декогеренции.

Важно также отметить, что эти процессы подчиняются уравнению Шрёдингера, описывающему систему «измеритель+система», и они — локальны (в смысле, не

нарушают причинность — разумеется, возмущение, вызванное взаимодействием с измерителем, не выходит за пределы светового конуса).

Наконец, как мы установили выше, оффдиагональные элементы матрицы плотности в каком-то смысле характеризуют степень «квантовости» нашей системы

поэтому мы выяснили, что в результате взаимодействия с окружающей средой, система как бы становится «классической».

Пусть теперь мы всё-таки узнали результат измерения — выяснили, что система находится в конкретном состоянии.

Матрица плотности уже диагональна, и для дальнейшего описания мы уже можем пользоваться классической интуицией.

Тогда, как и в классической статистике, мы можем учесть это знание

(говоря на языке теории вероятностей, вычислять

????

неравенство Белла

(подробно потом обсужу его)

неопределенность и измерения

откуда вообще она и как убедиться в этом?
и тут физический смысл, также ссылки на математику.
мб задачи порешаю.
еще там разные ее формы есть, например форма Вейля, через средние.
что за?
сивухин тоже про это писал много

пример измерений (??!!)

две неопределенности при измерениях??

(задача вроде из овочоса)
мы представляем себе измерение так:
при измерениях в систему вводится неконтролируемая неопределенность $\langle \Delta x_0^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$.

Далее из соотношений неопределенностей можно найти неопределенность, которая вносится в импульс:

$$\langle \Delta p_x^2 \rangle \geqslant \frac{\hbar^2}{2\langle \Delta x_0^2 \rangle} E$$

А из неопределенности импульса по формуле для равномерного движения к неопределенности в расстоянии:

$$\langle \Delta x_\tau^2 \rangle = \frac{\langle \Delta p_x^2 \rangle \tau^2}{m^2} \geqslant \frac{\hbar^2 \tau^2}{4m^2 \langle \Delta x_0^2 \rangle}$$

Получается, что спустя $\Delta\tau$ после измерения, дисперсия конечной координаты $\langle \Delta x^2 \rangle$ будет состоять из ДВУХ дисперсий:

$$\langle \Delta x^2 \rangle \geqslant \langle \Delta x_0^2 \rangle + \frac{\hbar^2 \tau^2}{4m^2 \langle \Delta x_0^2 \rangle}$$

получается, что неопределенность измерения первой координаты, таким вот образом меняет неопределенность в пути.

!! таким образом частица может смешаться при измерении на минимальное расстояние $\langle \Delta x^2 \rangle_{min} = \hbar\tau/m$
кстатиати, если у нас действует сила, то от нее смещение будет $\frac{F\tau^2}{2m}$.
таким образом ее зарегистрировать можно, если

$$\frac{F\tau^2}{2m} \geqslant \hbar\tau/m$$

так и можно узнать, какую минимальную силу за данное время можно поменить.

заметим, что за малое время на самом деле силу поменить не получится, так как ее воздействие будет не достаточное для прорыва сквозь неопределенность.

Измерение

Вероятность координаты быть в $z_1 < z < z_2$

$$P(z_1 < z < z_2) = \int int \int_{z_1}^{z_2} |\psi(x,y,z)|^2 dxdydz$$

И эту формулу следует использовать для решения, если еще есть условие на импульс, чтобы это сделать перейдем в импульсное представление: $\psi(x,p_y,z) = \int dy e^{-iyp_y/\hbar}\psi(x,y,z), \qquad \psi^*(x,p_y,z) = \int dy e^{iyp_y/\hbar}\psi^*(x,y,z).$
нам нужно

$$|\psi(x,p_y,z)|^2 = \int\int dydy e^{-i(y-y)p_y/\hbar}\psi(x,y,z)\psi^*(x,y,z)$$

По итогу имеем:

$$P(z_1 < z < z_2, p_1 < p_y < p_2) = \int \int_{p_1}^{p_2} \int_{z_1}^{z_2} |\psi(x,p_y,z)|^2 \frac{dxdp_ydz}{2\pi\hbar}$$

проблема измерений

такая есть, ее и обсудим.

обзор

хз, чуть что - на вики пойти можно.

слабые измерения (?)

ну такое ест, мб дойду.

мотивация

см вики, там статья есть

обзор

In quantum mechanics (and computation and information), weak measurements are a type of quantum measurement that results in an observer obtaining very little information about the system on average, but also disturbs the state very little.[1]

From Busch's theorem[2] the system is necessarily disturbed by the measurement. In the literature weak measurements are also known as unsharp,[3] fuzzy,[3][4] dull, noisy,[5] approximate, and gentle[6] measurements. Additionally weak measurements are often confused with the distinct but related concept of the weak value.[7]

суть

хз, пока не актуально.

2.9.2 Simplified Theory of Measurements

Условие точного измерения (Киселев,???)

Выведите необходимое и достаточное условие точного измерения наблюдаемой F в дираковских обозначениях.

(Вопросы Киселева на развлечение (?!!!!!))

2.9.3 Quantum Entanglement

весь обзор ее тут будет, ибо как раз сдали посмотрим на все, что тут есть.

типичная модель

??

квантовая запутанность на километрах с помощью дронов

(интересно, но не актуально, мб когда-то буду добавлять)

Optical-Relayed Entanglement Distribution Using Dronesas Mobile Nodes Hua-YingLiu,Xiao-HuiTian,

Статья про квантовую запутанность на киллометры, создаю параграф про это и забиваю, ибо не актуально.

2.9.4 What Happens After Measurement?

Частица остается в том же состоянии, в котором мы ее измерили, или снова становятся такие же вероятности найти ее в разных состояниях до измерения? (?????)

(??? не знаю, нужно подумать про это хорошо!)

2.9.5 The Measurement Problem in Quantum Mechanics (???)

(там часто про это говорят, напишу потом. типа вообще непонятно, что такое измерение и открытые вопросы по поводу измерения, если все только квантовое.)

2.9.6 Quantum Zeno Effect

(all about it is here, see wiki or something for now)

2.9.7 Other About Measurements

(много вопросов еще есть про это.)

2.10 Measurement in QM: Other Ideas

(see note on quantum information for details)

2.10.1 The Perfect Measurement

(there are articles about it, I'll put them to the later part, and then I'll write about it here)

2.11 Mathematical Side of the Formalism of QM

(some other really conceptually important math concepts will also have some section here)

2.11.1 Reminder: Strict Definitions of Operators

We recall the standard notation and basic facts from the theory of selfadjoint operators on Hilbert spaces. Let $\mathscr{H}$ be a separable Hilbert space with an inner product $(,)$, which is complex-linear with respect to the first argument, and let A be a linear operator in $\mathscr{H}$ with the domain $D(A) \subseteq \mathscr{H}$ - a linear subset of $\mathscr{H}$. An operator A is called closed if its graph $\Gamma(A) = \{(\varphi, A\varphi) \in \mathscr{H} \times \mathscr{H} : \varphi \in D(A)\}$ is a closed subspace in $\mathscr{H} \times \mathscr{H}$. If the domain of A is dense [1] in $\mathscr{H}$, i.e., $\overline{D(A)} = \mathscr{H}$, the domain $D(A^*)$ of the adjoint operator A^* consists of $\varphi \in \mathscr{H}$ such that there is $\eta \in \mathscr{H}$ with the property that

$$(A\psi, \varphi) = (\psi, \eta) \quad \text{for all} \quad \psi \in D(A)$$

and the operator A^* is defined by $A^*\varphi = \eta$. An operator A is called symmetric if

$$(A\psi, \varphi) = (\psi, A\varphi) \quad \text{for all} \quad \varphi, \psi \in D(A)$$

By definition, the regular set of a closed operator A with a dense domain $D(A)$ is the set $\rho(A) = \{\lambda \in \mathbb{C} | A - \lambda I : D(A) \to \mathscr{H}$ is a bijection with a bounded inverse [2]$\}$, and for $\lambda \in \rho(A)$, the bounded operator $R_\lambda(A) = (A - \lambda I)^{-1}$ is called the resolvent of A at λ. The regular set $\rho(A) \subset \mathbb{C}$ is open and its complement $\sigma(A) = \mathbb{C} \backslash \rho(A)$ is the spectrum of A. The subset $\sigma_p(A)$ of $\sigma(A)$ consisting of eigenvalues of A of finite multiplicity is called the point spectrum.

An operator A is self-adjoint (or Hermitian) if $A = A^*$. Equivalently, A is symmetric and $D(A) = D(A^*)$, and for such operators $\sigma(A) \subset \mathbb{R}$. A symmetric operator A is called essentially self-adjoint if its closure $\bar{A} = A^{**}$ is self-adjoint. For a symmetric operator A the following conditions are equivalent:
(i) A is essentially self-adjoint.
(ii) $\operatorname{Ker}(A^* + iI) = \operatorname{Ker}(A^* - iI) = \{0\}$.
(iii) $\overline{\operatorname{Im}(A + iI)} = \overline{\operatorname{Im}(A - iI)} = \mathscr{H}$.

A symmetric operator A with $D(A) = \mathscr{H}$ is bounded and self-adjoint. An operator A is positive [3] if $(A\varphi, \varphi) \geq 0$ for all $\phi \in D(A)$, which we denote by $A \geq 0$. Positive operators satisfy the Cauchy-Bunyakovski-Schwarz inequality

$$|(A\varphi, \psi)|^2 \leq (A\varphi, \varphi)(A\psi, \psi) \quad \text{for all} \quad \varphi, \psi \in D(A) \tag{0.1}$$

In particular, $(A\varphi, \varphi) = 0$ implies that $A\varphi = 0$. Every bounded positive operator is self-adjoint [4]. We denote by $\mathscr{L}(\mathscr{H})$ the $\mathbb{C}^*$-algebra of bounded linear operators on $\mathscr{H}$ with the operator norm $\| \cdot \|$ and with the antiinvolution * given by the operator adjoint. Operator $A \in \mathscr{L}(\mathscr{H})$ is called compact if it maps bounded sets in $\mathscr{H}$ into pre-compact sets [5]. The vector space $\mathscr{C}(\mathscr{H})$ of compact operators on $\mathscr{H}$ is a closed two-sided ideal [6] of the $\mathbb{C}^*$-algebra $\mathscr{L}(\mathscr{H})$.

An operator $A \in \mathscr{C}(\mathscr{H})$ is of trace class if

$$\|A\|_1 = \sum_{n=1}^{\infty} \mu_n(A) < \infty$$

[01] We consider only linear operators with dense domains.
[2] By the closed graph theorem, the last condition is redundant.

where $\mu_n(A)$ are singular values of $A : \mu_n(A) = \sqrt{\lambda_n(A)} \geq 0$, where $\lambda_n(A)$ are eigenvalues of A^*A. Equivalently, an operator $A \in \mathscr{L}(\mathscr{H})$ is of trace class if and only if for every orthonormal basis $\{e_n\}_{n=1}^{\infty}$ for $\mathscr{H}$

$$\sum_{n=1}^{\infty} |(Ae_n, e_n)| < \infty$$

Since a permutation of an orthonormal basis is again an orthonormal basis, this condition can be replaced by

$$\sum_{n=1}^{\infty} (Ae_n, e_n) < \infty$$

for every orthonormal basis $\{e_n\}_{n=1}^{\infty}$ for $\mathscr{H}$. The trace of a trace class operator A is defined by

$$\operatorname{Tr} A = \sum_{n=1}^{\infty} (Ae_n, e_n)$$

and does not depend on the choice of an orthonormal basis $\{e_n\}_{n=1}^{\infty}$ for $\mathscr{H}$. A positive operator $A \in \mathscr{L}(\mathscr{H})$ is of trace class if

$$\sum_{n=1}^{\infty} (Ae_n, e_n) < \infty$$

for some orthonormal basis $\{e_n\}_{n=1}^{\infty}$ for $\mathscr{H}$. The space $\mathscr{S}_1$ of trace class operators in $\mathscr{H}$ is a Banach algebra with the norm $\|A\|_1 = \operatorname{Tr} \sqrt{A^*A}$, and is a two-sided ideal (von Neumann-Schatten ideal) in the $\mathbb{C}^*$-algebra $\mathscr{L}(\mathscr{H})$.

The property

$$\operatorname{Tr} AB = \operatorname{Tr} BA \quad \text{for all} \quad A \in \mathscr{S}_1, B \in \mathscr{L}(\mathscr{H})$$

is called the cyclic property of the trace. If $A \in \mathscr{S}_1$, the mapping $l_A(B) = \operatorname{Tr} AB, B \in \mathscr{L}(\mathscr{H})$, is a continuous linear functional on $\mathscr{L}(\mathscr{H})$, so that $\mathscr{S}_1 \subset \mathscr{L}(\mathscr{H})^*$ - the dual Banach space to $\mathscr{L}(\mathscr{H})$. However, $\mathscr{S}_1 \neq \mathscr{L}(\mathscr{H})^*$, but rather $\mathscr{S}_1 = \mathscr{C}(\mathscr{H})^*$, and the mapping $A \mapsto l_A$ is an isomorphism of Banach spaces. Similarly, the mapping $B \mapsto l_B$ gives an isomorphism $\mathscr{L}(\mathscr{H}) = \mathscr{S}_1^*$.

An operator $A \in \mathscr{L}(\mathscr{H})$ is called a Hilbert-Schmidt operator if $AA^* \in \mathscr{S}_1$. Equivalently, an operator $A \in \mathscr{L}(\mathscr{H})$ is a Hilbert-Schmidt operator if and only if for some orthonormal basis $\{e_n\}_{n=1}^{\infty}$ for $\mathscr{H}$

$$\sum_{n=1}^{\infty} \|Ae_n\|^2 < \infty$$

The vector space $\mathscr{S}_2$ of Hilbert-Schmidt operators in $\mathscr{H}$ is a Hilbert space with the inner product $(A, B)_2 = \operatorname{Tr} AB^*$. The Hilbert-Schmidt space $\mathscr{S}_2$ is also a two-sided ideal in the $\mathbb{C}^*$-algebra $\mathscr{L}(\mathscr{H})$.

2.11.2 Hilbert Space

(статья одна тут выгружена, мб посмотрю её, точно не скоро.)

[03] Non-negative, to be precise.
[4] This is true only for complex Hilbert spaces.
[5] The sets with compact closure.
[6] Ideal $\mathscr{C}(\mathscr{H})$ is the only closed two-sided ideal of $\mathscr{L}(\mathscr{H})$.

О важности строгого подхода к гильбертовым пространствам

(почему таким подходом вообще заниматься следует?)

основы гильбертова пространства

тупая обычная теория, потом напишу

2.11.3 Tensor Product of Hilbert Spaces

(наверное, по Нохриной это я писал, потому что нигде в других местах нет этой теории.)

Теория

Пусть пространства $\mathcal{H}_1$ и $\mathcal{H}_2$ - гильбертовы. Напомним, что гильбертовым называется полное евклидово пространство, то есть пространство со скалярным произведением, полное по норме, порожденной этим скалярным произведением. Для любых $\varphi \in \mathcal{H}_1$ и $\psi \in \mathcal{H}_2$ введём объект $\varphi \otimes \psi$. Определим сумму двух таких объектов и умножение этого объекта на произвольный комплексный скаляр так, чтобы

$$\alpha(\varphi \otimes \psi) = (\alpha\varphi) \otimes \psi = \varphi \otimes (\alpha\psi)$$
$$\forall \alpha \in \mathbb{C}, \varphi \in \mathcal{H}_1, \psi \in \mathcal{H}_2;$$
$$(\varphi_1 + \varphi_2) \otimes \psi = \varphi_1 \otimes \psi + \varphi_2 \otimes \psi$$
$$\forall \varphi_{1,2} \in \mathcal{H}_1, \psi \in \mathcal{H}_2;$$
$$\varphi \otimes (\psi_1 + \psi_2) = \varphi \otimes \psi_1 + \varphi \otimes \psi_2$$
$$\forall \varphi \in \mathcal{H}_1, \psi_{1,2} \in \mathcal{H}_2.$$

Пусть θ_1 нулевой вектор в $\mathcal{H}_1, \theta_2$ нулевой вектор в $\mathcal{H}_2$. Тогда $\forall \varphi_{1,2} \in \mathcal{H}_1$ и $\psi_{1,2} \in \mathcal{H}_2$ имеем

$$\theta_1 \otimes \psi_1 + \varphi_2 \otimes \psi_2 = (\varphi_2 - \varphi_2) \otimes \psi_1 + \varphi_2 \otimes \psi_2 =$$
$$= \varphi_2 \otimes \psi_1 - \varphi_2 \otimes \psi_1 + \varphi_2 \otimes \psi_2 = \varphi_2 \otimes (\psi_1 - \psi_1 + \psi_2) =$$
$$= \varphi_2 \otimes (\theta_2 + \psi_2) = \varphi_2 \otimes \psi_2$$

точно так же

$$\varphi_1 \otimes \psi_1 + \varphi_2 \otimes \theta_2 = \varphi_1 \otimes \psi_1 + \varphi_2 \otimes (\psi_1 - \psi_1) =$$
$$= \varphi_1 \otimes \psi_1 + \varphi_2 \otimes \psi_1 - \varphi_2 \otimes \psi_1 = (\varphi_1 + \varphi_2 - \varphi_2) \otimes \psi_1 =$$
$$= (\varphi_1 + \theta_1) \otimes \psi_1 = \varphi_1 \otimes \psi_1.$$

Таким образом, обьекты $\theta_1 \otimes \psi_1$ и $\varphi_1 \otimes \theta_2$ играют роль нуля в линейном пространстве L всевозможных конечных линейных комбинаций объектов $\varphi \otimes \psi$, то есть

$$L = \left\{ \sum_{i,j=1}^{N} \alpha_{ij} \varphi_i \otimes \psi_j | N \in \mathbb{N}, \right.$$
$$\left. \alpha_{ij} \in \mathbb{C}, \varphi_1 ... \varphi_N \in \mathcal{H}_1, \psi_1 ... \psi_N \in \mathcal{H}_2 \right\}.$$

Выражения (1) - (3) вместе с определением нуля $\theta_1 \otimes \psi_1$ и $\varphi_1 \otimes \theta_2$ задают линейную структуру на множестве L.

Введем на L скалярное произведение. Для этого сначала определим произведение для объектов $\varphi \otimes \psi$ следующим образом: $\forall \varphi_{1,2} \in \mathcal{H}_1$ и $\forall \psi_{1,2} \in \mathcal{H}_2$,

$$(\varphi_1 \otimes \psi_1, \varphi_2 \otimes \psi_2) = (\varphi_1, \varphi_2)(\psi_1, \psi_2)$$

ТОГДа ДлЯ

$$\Psi = \sum_{i,j=1}^{N} \alpha_{ij} \varphi_i \otimes \psi_j \in L, \quad \text{и}$$

$$\tilde{\Psi} = \sum_{k,l=1}^{N} \beta_{kl} \tilde{\varphi}_k \otimes \tilde{\psi}_l \in L$$

определим скалярное произведение элементов L как

$$(\Psi, \tilde{\Psi}) = \sum_{i,j=1}^{N} \sum_{k,l=1}^{N} \alpha_{ij} \beta_{kl} \left(\varphi_i \otimes \psi_j, \tilde{\varphi}_k \otimes \tilde{\psi}_l \right).$$

Упражнение. Докажите корректность такого определения. Таким образом, мы получили линейное евклидово пространство.

Определение 1. Тензорным произведением $\mathcal{H}_1 \otimes \mathcal{H}_2$ двух гильбертовых пространств $\mathcal{H}_1$ и $\mathcal{H}_2$ называется пополнение множества всех возможных конечных линейных комбинаций $\varphi \otimes \psi$ по норме, порожденной скалярным произведением (7).

Если мы работаем с тензорным произведением бесконечномерных пространств, то множество всех конечных линейных комбинаций не полно. Поэтому для того, чтобы тензорное произведение было также гильбертовым пространством, необходимо 6 его пополнить. Нередко в квантовой механике работают с тензорным произведением конечномерных гильбертовых пространств, изоморфных $\mathbb{C}^n, n \in \mathbb{N}$. В этом случае конечные линейные комбинации образуют полное пространство, и процедуры пополнения не требуется. в гильбертовых $\mathcal{H}_1$ и $\mathcal{H}_2$ соответственно, то $\varphi_i \otimes \psi_j$ - ортонормированный базис в тензорном произведении $\mathcal{H}_1 \otimes \mathcal{H}_2$.

Доказательство. Базис - это полная ортогональная система. Полнота обеспечивает приближение произвольного элемента с любой точностью (по норме пространства), а ортогональность обеспечивает единственность коэффициентов разложения. Поскольку ортонормированность $\varphi_i \otimes \psi_j$ очевидна, нам нужно доказать лишь полноту. Возьмём произвольный вектор $\varphi \otimes \psi$. Вектор φ раскладывается по базису φ_i, а ψ - по ψ_j: $\varphi = \sum\limits_{i=1}^{+\infty} c_i \varphi_i$ и $\psi = \sum\limits_{j=1}^{+\infty} d_j \psi_j$. Здесь по равенству Парсеваля выполнено $\sum\limits_{i=1}^{+\infty} |c_i|^2 < +\infty$, $\sum\limits_{j=1}^{+\infty} |d_j|^2 < +\infty$ и, следовательно, верно $\sum\limits_{i,j=1}^{+\infty} |c_i d_j|^2 \leq \sum\limits_{i=1}^{+\infty} |c_i|^2 \sum\limits_{j=1}^{+\infty} |d_j|^2 < +\infty$. Значит, существует вектор $\alpha = \sum\limits_{i,j=1}^{+\infty} c_i d_j \varphi_i \otimes \psi_j$. Покажем, что

$$\left\| \varphi \otimes \psi - \sum_{i,j=1}^{M,N} c_i d_j \varphi_i \otimes \psi_j \right\| \to 0$$

при $M, N \to +\infty$. Рассмотрим следующие частичные суммы:

$$f_M = \sum_{i=1}^{M} c_i \varphi_i, \quad g_N = \sum_{j=1}^{N} d_j \psi_j$$

Тензорное произведение частичных сумм

$$f_M \otimes g_N = \sum_{i,j=1}^{M,N} c_i d_j \varphi_i \otimes \psi_j$$

Рассмотрим цепочку неравенств:

$$\|\varphi\otimes\psi - f_M\otimes g_N\| =$$
$$= \left\|\varphi\otimes\psi \pm \frac{1}{2}f_M\otimes\psi \pm \frac{1}{2}\varphi\otimes g_N - f_M\otimes g_N\right\| \leq$$
$$\leq \frac{1}{2}\|\varphi\otimes(\psi-g_N)+(\varphi-f_M)\otimes\psi+$$
$$+f_M\otimes(\psi-g_N)+(\varphi-f_M)\otimes g_N\| \leq$$
$$\leq \frac{1}{2}\left(\|\varphi\|\,\|\psi-g_N\|+\|\varphi-f_M\|\,\|\psi\|+\right.$$
$$\left.+\|f_M\|\,\|\psi-g_N\|+\|\varphi-f_M\|\,\|g_N\|\right)\to 0$$

при $M,N\to+\infty$. Пример 3. Рассмотрим тензорное произведение $\mathbb{C}^2\otimes\mathbb{C}^2$. Базисом в тензорном произведении являются в соответствии с Утверждением 2 следующие векторы:

$$\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix},\quad \begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix},$$
$$\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix},\quad \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}.$$

Как правило, гораздо удобнее работать именно с такими объектами. Тем не менее часто в физической литературе принято использовать пространства, изоморфные тензорному произведению. Напомним, что изоморфизм - это взаимно однозначное отображение на пространство. Для задания такого отображения достаточно определить отображение базисных векторов. В нашем примере пространство $\mathbb{C}^2\otimes\mathbb{C}^2$ является четырёхмерным, поэтому естественно отобразить его на $\mathbb{C}^4$. Зададим изоморфизм (изометрический) U : $\mathbb{C}^2\otimes\mathbb{C}^2\to\mathbb{C}^4$:

$$U\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}=\begin{pmatrix}1\\0\\0\\0\end{pmatrix},\quad U\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}=\begin{pmatrix}0\\1\\0\\0\end{pmatrix}$$

8 и так далее. Такое отображение реализует кронекерово произведение. Необходимо заметить, что оно не единственно. Более того, в нем нет необходимости - работать можно в исходном тензорном произведении пространств.

Пусть в каждом из гильбертовых пространств заданы операторы $\hat{S}$: $D(\hat{S})\to\mathcal{H}_1$ и $\hat{T}$: $D(\hat{T})\to\mathcal{H}_2$. Здесь области определения операторов $-D(\hat{S})\subset\mathcal{H}_1$ и $D(\hat{T})\subset\mathcal{H}_2$ соответственно. Тензорным произведением этих операторов называется оператор $\hat{T}\otimes\hat{S}$, действие которого для любых $\varphi\in D(\hat{S})$ и $\psi\in D(\hat{T})$ определено следующим образом: $(\hat{T}\otimes\hat{S})(\varphi\otimes\psi)=(\hat{T}\varphi)\otimes(\hat{S}\psi)$. Т.е. первый оператор действует только на первый вектор, а второй - только на второй. Соответственно, $\forall\varphi_1...\varphi_N\in D(\hat{S})$ и $\forall\psi_1...\psi_N\in D(\hat{T})$ действие оператора $\hat{S}\otimes\hat{T}$ на линейную комбинацию тензорного произведения векторов опеределно как

$$(\hat{S}\otimes\hat{T})\left(\sum_{i,j=1}^{N}a_{ij}\varphi_i\otimes\psi_j\right)=\sum_{i,j=1}^{N}a_{ij}(\hat{S}\otimes\hat{T})\,(\varphi_i\otimes\psi_j)$$

Хочется определить тензорное произведение операторов на произвольном объекте $\Psi\in\mathcal{H}_1\otimes\mathcal{H}_2$. Произвольный элемент тензорного произведения бесконечномерных пространств является пределом частичных сумм

$$\Psi=\lim_{N\to+\infty}\sum_{n=1}^{N}c_n\psi_n,$$

где $\{\psi_n\}$ - базис в сепарабельном гильбертовом пространстве. Для определения действия тензорного произведения операторов на такой объект необходимо продолжить действие по непрерывности. Но неограниченный оператор $\hat{S}$ является всюду разрывным, поэтому нельзя определить действие оператора на предел частичных сумм по непрерывности. Тем не менее если оператор $\hat{S}$ самосопряженный, то такой переход верен. Покажем это для случая, когда каждый из операторов $\hat{S}$ и $\hat{T}$ обладает только точечным спектром и, значит, базисом из собственных функций. Для сложения моментов этого достаточно.

Рассмотрим $\psi \in D(\hat{S})$. Пусть $\{\psi_n\}$ - базис из собственных 9 функций $\hat{S}$ в $\mathcal{H}_1$. Вектор ψ раскладывается по базису

$$\psi = \sum_n c_n \psi_n$$

Мы не можем напрямую записать действие оператора $\hat{S}$ на этот вектор как предел частичных сумм, на каждый член которой действует $\hat{S}$ из-за разрывности $\hat{S}$. Так как $\psi \in D(\hat{S})$, то $\hat{S}\psi \in \mathcal{H}_1$. Вектор $\hat{S}\psi$ может быть разложен по базису ψ_n:

$$\hat{S}\psi = \sum_n d_n \psi_n$$

где коэффициенты Фурье d_n определяются выражением

$$d_n = \left(\psi_n, \hat{S}\psi\right) = \left(\hat{S}\psi_n, \psi\right) = \lambda_n \left(\psi_n, \psi\right)$$

Значит,

$$\hat{S}\psi = \sum_n d_n \psi_n = \sum_n \lambda_n c_n \psi_n$$

Таким образом, мы показали, что

$$\hat{S}\psi = \sum_n \lambda_n c_n \psi_n$$

Определение 4. Тензорным произведением двух самосопряженных операторов $\hat{S} : D(\hat{S}) \to \mathcal{H}_1$ и $\hat{T} : D(\hat{T}) \to \mathcal{H}_2$, каждый из которых обладает чисто точечным спектром λ_n и μ_m и, значит, базисом из собственных функций $\{\varphi_n\}$ и $\{\psi_m\}$ соответственно, называется оператор $\hat{S} \otimes \hat{T}$, действие которого на

$$\Psi \in D(\hat{S} \otimes \hat{T}) =$$

$$= \left\{ \Psi \in \mathcal{H}_1 \otimes \mathcal{H}_2 \left| \sum_n \sum_m \right| \lambda_n \Big|^2 |\mu_m|^2 |\alpha_{nm}|^2 < +\infty \right\}$$

определяется как

$$(\hat{S} \otimes \hat{T})\Psi = \sum_n \sum_m \lambda_n \mu_m \alpha_{nm} \varphi_n \otimes \psi_m$$

Здесь вектор Ψ разложен по базису в $\mathcal{H}_1 \otimes \mathcal{H}_2$:

$$\Psi = \sum_n \sum_m \alpha_{nm} \varphi_n \otimes \psi_m$$

Область определения 10 задется очень естественным требованием, чтобы вектор $(\hat{S} \otimes \hat{T})\Psi$ лежал в пространстве $\mathcal{H}_1 \otimes \mathcal{H}_2$. Упражнение. Покажите, что $(\hat{S} \otimes \hat{T})\Psi \in \mathcal{H}_1 \otimes \mathcal{H}_2$ тогда и только тогда, когда $\Psi \in D(\hat{S} \otimes \hat{T})$, определенную выражением (10)

В дальнейшем нам понадобится более простое определение определение тензорного произведения операторов в конечномерном пространстве.

Определение 5. Тензорным произведением двух самосопряженных операторов $\hat{S}$ и $\hat{T}$ в конечномерных $\mathcal{H}_1$ и $\mathcal{H}_2$ называется оператор $\hat{S} \otimes \hat{T}$, действие которого на объект $\Psi \in \mathcal{H}_1 \otimes \mathcal{H}_2$ задается выражением (9).

Замечание 6. Пусть два симметрических оператора $\hat{S}$ и $\hat{T}$ действут на конечномерных гильбертовых пространствах $\mathbb{C}^n$ и $\mathbb{C}^m$ соответственно. Пусть в $\mathbb{C}^n$ Задан ортонормированный базис $\{\varphi_i\}, i = \overline{1,n}$, а в $\mathbb{C}^m$ - базис $\{\psi_j\}, j = \overline{1,m}$. Каждый из этих операторов в заданном базисе можно записать в виде матрицы с компонентами:

$$S_{ij} = \left(\varphi_i, \hat{S}\varphi_j\right), T_{kl} = \left(\psi_k, \hat{T}\psi_l\right)$$

Задавая на этом базисе какой-либо изометрический изоморфизм $U : \mathbb{C}^n \otimes \mathbb{C}^m \to \mathbb{C}^{n \cdot m}$, реализуемый как $\varphi_i \otimes \psi_k \cong \Psi_{s_{ik}}$, где $s = \overline{1, n \cdot m}$. Мы можем задать на $\mathbb{C}^{n \cdot m}$ оператор $\hat{W} \cong \hat{S} \otimes \hat{T}$ матрицей:

$$W_{s_{ik}s_{jl}} = \left(\Psi_{s_{ik}}, \hat{W}\Psi_{s_{jl}}\right) = \left(\varphi_i \otimes \psi_k, (\hat{S} \otimes \hat{T})\varphi_j \otimes \psi_l\right) =$$

У пражнение. Пусть изоморфизм U осуществляется как:

$$\left(\Psi_{s_{ik}}\right)_a = \left(\varphi_i\right)_b \cdot \left(\psi_k\right)_c$$

11 где $\left(\Psi_{s_{ik}}\right)_a$ это a компонента вектора $\Psi_{s_{ik}}$, а $\left(\varphi_i\right)_b$ это b компонента вектора φ_i. Здесь $b = \overline{1,n}, c = \overline{1,m}$, а $a = b + (c-1) \cdot n$. Покажите, что тензорное произведение операторов осуществляется как кронекерово произведение матриц.

Таким образом, кронекерово произведение лишь одна удобная реализация тензорного произведения, задаваемая конкретным отображением U.

Тензорное произведение гильбертовых пространств обеспечивает естественный математический аппарат для описания в квантовой механике независимых величин. Рассмотрим две наблюдаемые A и B, которым соответствуют самосопряженные операторы $\hat{A}$ и $\hat{B}$, каждый из которых действует в своем гильбертовом пространстве. Пусть величины A и B независимы. В силу структуры тензорного произведения оператор $\hat{A} \otimes \hat{B}$ имеет независимые вероятностные характеристики в состоянии $\Psi = \psi \otimes \varphi$. Например, среднее значение

$$\langle \hat{A} \otimes \hat{B} \rangle_\Psi = (\psi, \hat{A}\psi)(\varphi, \hat{B}\varphi) = \langle \hat{A} \rangle_\psi \langle \hat{B} \rangle_\varphi$$

Значит, тензорное произведение гильбертовых пространств корректно описывает совместные распределения независимых величин Пример 9. Рассмотрим пример с трехмерным изотропным осциллятором. Так как энергии колебаний по каждой из осей такой системы не зависят от колебаний по другим осям, то естественно описывать состояние трехмерного осциллятора в тензорном произведении гильбертовых пространств, каждое их которых используется для описания одномерного осциллятора. В силу того что гамильтониан распадается на сумму трех гамильтонианов одномерного осциллятора по независимым переменным, естественно записать его в виде

$$\hat{H} = \hat{H}_x \otimes \hat{E} \otimes \hat{E} + \hat{E} \otimes \hat{H}_y \otimes \hat{E} + \hat{E} \otimes \hat{E} \otimes \hat{H}_z.$$

Этот оператор действует в тензорном произведении пространств: $\mathcal{H}_1 = L^2(\mathbb{R}) \otimes L^2(\mathbb{R}) \otimes L^2(\mathbb{R})$. Базисом из собственных векторов этого гамильтониана является набор

$$\psi_{n_1} \otimes \psi_{n_2} \otimes \psi_{n_3}$$

Может быть построен так называемый естественный изоморфизм [1]$U : \mathcal{H}_1 \to \mathcal{H}_2$, где $\mathcal{H}_2 = L^2(\mathbb{R}^3)$:

$$U(\psi_{n_1} \otimes \psi_{n_2} \otimes \psi_{n_3}) \to \psi_{n_1}(x)\psi_{n_2}(y)\psi_{n_3}(z).$$

Пример 10. Тензорное произведение в линейной алгебре. Рассмотрим пространство $\mathbb{R}^3$. Определим в нем вектор как тройку чисел a_i (его координат в определенном ортонормированном базисе $\mathbf{e}_i$), которые при поворотах базисных векторов в $\mathbb{R}^3$, задаваемых матрицей R с компонентами $R_{ij}, i, j = 1, 2, 3$, преобразуются как $a'_i = R_{ij}a_j$. Тогда можно определить тензорное произведение векторов $\mathbf{a}$ и $\mathbf{b}$:

$$\mathbf{a} \otimes \mathbf{b} = \sum_{i,j=1}^{3} a_i b_j \mathbf{e}_i \otimes \mathbf{e}_j.$$

Координаты этого объекта $a_i b_j$ преобразуются как

$$a'_i b'_j = R_{il} R_{jm} a_l b_m.$$

Это пример простейшего тензора.

2.12 Classical Mechanics for QM

We assume that the reader is familiar with the basic notions from the theory of smooth (that is, C^∞) manifolds and recall here the standard notation. Unless it is stated explicitly otherwise, all maps are assumed to be smooth and all functions are assumed to be smooth and real-valued. Local coordinates $\boldsymbol{q} = (q^1, ..., q^n)$ on a smooth n-dimensional manifold M at a point $q \in M$ are Cartesian coordinates on $\varphi(U) \subset \mathbb{R}^n$, where (U, φ) is a coordinate chart on M centered at $q \in U$. For $f : U \to \mathbb{R}^n$ we denote $(f \circ \varphi^{-1})(q^1, ..., q^n)$ by $f(\boldsymbol{q})$, and we let

$$\frac{\partial f}{\partial \boldsymbol{q}} = \left(\frac{\partial f}{\partial q^1}, ..., \frac{\partial f}{\partial q^n} \right)$$

stand for the gradient of a function f at a point $\boldsymbol{q} \in \mathbb{R}^n$ with Cartesian coordinates $(q^1, ..., q^n)$. We denote by

$$\mathcal{A}^\bullet(M) = \bigoplus_{k=0}^{n} \mathcal{A}^k(M)$$

the graded algebra of smooth differential forms on M with respect to the wedge product, and by d the de Rham differential - a graded derivation of $\mathcal{A}^\bullet(M)$ of degree 1 such that df is a differential of a function $f \in \mathcal{A}^0(M) = C^\infty(M)$. Let $\mathrm{Vect}(M)$ be the Lie algebra of smooth vector fields on M with the Lie bracket [,], given by a commutator of vector fields. For $X \in \mathrm{Vect}(M)$ we denote by $\mathcal{L}_X$ and i_X, respectively, the Lie derivative along X and the inner product with X. The Lie derivative is a degree 0 derivation of $\mathcal{A}^\bullet(M)$ which commutes with d and satisfies $\mathcal{L}_X(f) = X(f)$ for $f \in \mathcal{A}^0(M)$, and the inner product is a degree -1 derivation of $\mathcal{A}^\bullet(M)$ satisfying $i_X(f) = 0$
and $i_X(df) = X(f)$ for $f \in \mathcal{A}^0(M)$. They satisfy Cartan formulas

$$\mathcal{L}_X = i_X \circ d + d \circ i_X = (d + i_X)^2$$
$$i_{[X,Y]} = \mathcal{L}_X \circ i_Y - i_Y \circ \mathcal{L}_X$$

For a smooth mapping of manifolds $f : M \to N$ we denote by $f_* : TM \to TN$ and $f^* : T^*N \to T^*M$, respectively, the induced mappings on tangent and cotangent bundles. Other notations, including those traditional for classical mechanics, will be introduced in the main text.

2.12.1 1. Classical Lagrangian Mechanics for QM

1.1. Generalized coordinates.

Classical mechanics describes systems of finitely many interacting particles [1]. A system is called closed if its particles do not interact with the outside material bodies. The position of a system in space is specified by positions of its particles and defines a point in a smooth, finite-dimensional manifold M, the configuration space of a system. Coordinates on M are called generalized coordinates of a system, and the dimension $n = \dim M$ is called the number of degrees of freedom [2].

The state of a system at any instant of time is described by a point $q \in M$ and by a tangent vector $v \in T_qM$ at this point. The basic principle of classical mechanics is the Newton-Laplace determinacy principle which asserts that a state of a system at a given instant completely determines its motion at all times t (in the future and in the past). The motion is described by the classical trajectory - a path $\gamma(t)$ in the configuration space M. In generalized coordinates $\gamma(t) = (q^1(t), ..., q^n(t))$, and corresponding derivatives $\dot{q}^i = \frac{dq^i}{dt}$ are called generalized velocities. The Newton-Laplace principle is a fundamental experimental fact confirmed by our perception of everyday experiences. It implies that generalized accelerations $\ddot{q}^i = \frac{d^2q^i}{dt^2}$ are uniquely defined by generalized coordinates q^i and generalized velocities $\dot{q}^i$, so that classical trajectories satisfy a system of second order ordinary differential equations, called equations of motion. In the next section we formulate the most general principle governing the motion of mechanical systems.
1.2. The principle of the least action. A Lagrangian system on a configuration space M is defined by a smooth, real-valued function L on $TM \times \mathbb{R}$ - the direct product of a tangent bundle TM of M and the time axis [3] called the Lagrangian function (or simply, Lagrangian). The motion of a

Lagrangian system (M, L) is described by the principle of the least action in the configuration space (or Hamilton's principle), formulated as follows.

Let

$$P(M)_{q_0,t_0}^{q_1,t_1} = \{\gamma : [t_0, t_1] \to M; \gamma(t_0) = q_0, \gamma(t_1) = q_1\}$$

be the space of smooth parametrized paths in M connecting points q_0 and q_1. The path space $P(M) = P(M)_{q_0,t_0}^{q_1,t_1}$ is an infinite-dimensional real Frchet manifold, and the tangent space $T_\gamma P(M)$ to $P(M)$ at $\gamma \in P(M)$ consists of all smooth vector fields along the path γ in M which vanish at the endpoints q_0 and q_1. A smooth path Γ in $P(M)$, passing through $\gamma \in P(M)$, is called a variation with fixed ends of the path $\gamma(t)$ in M. A variation Γ is a family $\gamma_\varepsilon(t) = \Gamma(t, \varepsilon)$ of paths in M given by a smooth map

$$\Gamma : [t_0, t_1] \times [-\varepsilon_0, \varepsilon_0] \to M$$

such that $\Gamma(t, 0) = \gamma(t)$ for $t_0 \le t \le t_1$ and $\Gamma(t_0, \varepsilon) = q_0, \Gamma(t_1, \varepsilon) = q_1$ for $-\varepsilon_0 \le \varepsilon \le \varepsilon_0$. The tangent vector

$$\delta\gamma = \left.\frac{\partial\Gamma}{\partial\varepsilon}\right|_{\varepsilon=0} \in T_\gamma P(M)$$

corresponding to a variation $\gamma_\varepsilon(t)$ is traditionally called an infinitesimal variation. Explicitly,

$$\delta\gamma(t) = \Gamma_* \left(\frac{\partial}{\partial\varepsilon}\right)(t, 0) \in T_{\gamma(t)}M, \quad t_0 \le t \le t_1,$$

[01] A particle is a material body whose dimensions may be neglected in describing its motion.
[2] Systems with infinitely many degrees of freedom are described by classical field theory.
[3] It follows from the Newton-Laplace principle that L could depend only on generalized coordinates and velocities, and on time.

where $\frac{\partial}{\partial\varepsilon}$ is a tangent vector to the interval $[-\varepsilon_0, \varepsilon_0]$ at 0 . Finally, a tangential lift of a path $\gamma : [t_0, t_1] \to M$ is the path $\gamma' : [t_0, t_1] \to TM$ defined by $\gamma'(t) = \gamma_* \left(\frac{\partial}{\partial t}\right) \in T_{\gamma(t)}M, t_0 \leq t \leq t_1$, where $\frac{\partial}{\partial t}$ is a tangent vector to $[t_0, t_1]$ at t. In other words, $\gamma'(t)$ is the velocity vector of a path $\gamma(t)$ at time t.

Definition. The action functional $S : P(M) \to \mathbb{R}$ of a Lagrangian system (M, L) is defined by

$$S(\gamma) = \int_{t_0}^{t_1} L\left(\gamma'(t), t\right) dt$$

Principle of the Least Action (Hamilton's principle). A path $\gamma \in PM$ describes the motion of a Lagrangian system (M, L) between the position $q_0 \in M$ at time t_0 and the position $q_1 \in M$ at time t_1 if and only if it is a critical point of the action functional S,

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} S\left(\gamma_\varepsilon\right) = 0$$

for all variations $\gamma_\varepsilon(t)$ of $\gamma(t)$ with fixed ends.
The critical points of the action functional are called extremals and the principle of the least action states that a Lagrangian system (M, L)
moves along the extremals [4]. The extremals are characterized by equations of motion - a system of second order differential equations in local coordinates on TM. The equations of motion have the most elegant form for the following choice of local coordinates on TM.

Definition. Let (U, φ) be a coordinate chart on M with local coordinates $\boldsymbol{q} = (q^1, ..., q^n)$. Coordinates

$$(\boldsymbol{q}, \boldsymbol{v}) = \left(q^1, ..., q^n, v^1, ..., v^n\right)$$

on a chart TU on TM, where $\boldsymbol{v} = (v^1, ..., v^n)$ are coordinates in the fiber corresponding to the basis $\frac{\partial}{\partial q^1}, ..., \frac{\partial}{\partial q^n}$ for T_qM, are called standard coordinates.
Standard coordinates are Cartesian coordinates on $\varphi_*(TU) \subset T\mathbb{R}^n \simeq \mathbb{R}^n \times \mathbb{R}^n$ and have the property that for $(q, v) \in TU$ and $f \in C^\infty(U)$,

$$v(f) = \sum_{i=1}^{n} v^i \frac{\partial f}{\partial q^i} = \boldsymbol{v}\frac{\partial f}{\partial \boldsymbol{q}}.$$

Let (U, φ) and (U', φ') be coordinate charts on M with the transition functions $F = (F^1, ..., F^n) = \varphi' \circ \varphi^{-1} : \varphi\left(U \cap U'\right) \to \varphi'\left(U \cap U'\right)$, and let $(\boldsymbol{q}, \boldsymbol{v})$ and $(\boldsymbol{q}', \boldsymbol{v}')$, respectively, be the standard coordinates on TU and TU'. We have $\boldsymbol{q}' = F(\boldsymbol{q})$ and $\boldsymbol{v}' = F_*(\boldsymbol{q})\boldsymbol{v}$, where $F_*(\boldsymbol{q}) = \left\{\frac{\partial F^i}{\partial q^j}(\boldsymbol{q})\right\}_{i,j=1}^{n}$ is a matrixvalued function on $\varphi\left(U \cap U'\right)$. Thus "vertical" coordinates $\boldsymbol{v} = (v^1, ..., v^n)$ in the fibers of $TM \to M$ transform like components of a tangent vector on M under the change of coordinates on M.
The tangential lift $\gamma'(t)$ of a path $\gamma(t)$ in M in standard coordinates on TU is $(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t)) = (q^1(t), ..., q^n(t), \dot{q}^1(t), ..., \dot{q}^n(t))$, where the dot stands for the time derivative, so that

$$L\left(\gamma'(t), t\right) = L(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t).$$

Following a centuries long tradition [5], we will usually denote standard coordinates by

$$(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \left(q^1, ..., q^n, \dot{q}^1, ..., \dot{q}^n\right)$$

where the dot does not stand for the time derivative. Since we only consider paths in TM that are tangential lifts of paths in M, there will be no confusion [6].

Theorem 1.1. The equations of motion of a Lagrangian system (M, L) in standard coordinates on TM are given by the Euler-Lagrange equations

$$\frac{\partial L}{\partial \boldsymbol{q}}(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t)\right) = 0.$$

Proof. Suppose first that an extremal $\gamma(t)$ lies in a coordinate chart U of M. Then a simple computation in standard coordinates, using integration by parts, gives

$$\begin{aligned}
0 &= \left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} S\left(\gamma_\varepsilon\right) \\
&= \left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \int_{t_0}^{t_1} L(\boldsymbol{q}(t,\varepsilon), \dot{\boldsymbol{q}}(t,\varepsilon), t) dt \\
&= \sum_{i=1}^{n} \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q^i}\delta q^i + \frac{\partial L}{\partial \dot{q}^i}\delta \dot{q}^i\right) dt \\
&= \sum_{i=1}^{n} \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\right) \delta q^i dt + \sum_{i=1}^{n} \left.\frac{\partial L}{\partial \dot{q}^i}\delta q^i\right|_{t_0}^{t_1}.
\end{aligned}$$

The second sum in the last line vanishes due to the property $\delta q^i\left(t_0\right) = \delta q^i\left(t_1\right) = 0, i = 1, ..., n$. The first sum is zero for arbitrary smooth functions δq^i on the interval $[t_0, t_1]$ which vanish at the endpoints. This implies that for each term in the sum the integrand is identically zero,

$$\frac{\partial L}{\partial q^i}(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t)\right) = 0, \quad i = 1, ..., n.$$

Since the restriction of an extremal of the action functional S to a coordinate chart on M is again an extremal, each extremal in standard coordinates on TM satisfies Euler-Lagrange equations.

Remark. In calculus of variations, the directional derivative of a functional S with respect to a tangent vector $V \in T_\gamma P(M)$ - the Gato derivative is defined by

$$\delta_V S = \left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} S\left(\gamma_\varepsilon\right),$$

where γ_ε is a path in $P(M)$ with a tangent vector V at $\gamma_0 = \gamma$. The result of the above computation (when γ lies in a coordinate chart $U \subset M$) can be written as

$$\begin{aligned}
\delta_V S &= \int_{t_0}^{t_1} \sum_{i=1}^{n} \left(\frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}\right)(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t) v^i(t) dt \\
&= \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial \boldsymbol{q}} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\boldsymbol{q}}}\right)(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t) \boldsymbol{v}(t) dt
\end{aligned} \tag{1.1}$$

[04] The principle of the least action does not state that an extremal connecting points q_0 and q_1 is a minimum of S, nor that such an extremal is unique. It also does not state that any two points can be connected by an extremal.

[5] Used in all texts on classical mechanics and theoretical physics.

[6] We reserve the notation $(\boldsymbol{q}(t), \boldsymbol{v}(t))$ for general paths in TM.

Here $V(t) = \sum_{i=1}^{n} v^i(t) \frac{\partial}{\partial q^i}$ is a vector field along the path γ in M. Formula (1.1) is called the formula for the first variation of the action with fixed ends. The principle of the least action is a statement that $\delta_V S(\gamma) = 0$ for all $V \in T_\gamma P(M)$.

Remark. It is also convenient to consider a space $\widehat{P(M)} = \{\gamma : [t_0, t_1] \to M\}$ of all smooth parametrized paths in M. The tangent space $T_\gamma \widehat{P(M)}$ to $\widehat{P(M)}$ at $\gamma \in \widehat{P(M)}$ is the space of all smooth vector fields along the path γ in M (no condition at the endpoints). The computation in the proof of Theorem 1.1 yields the following formula for the first variation of the action with free ends:

$$\delta_V S = \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial \boldsymbol{q}} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\boldsymbol{q}}} \right) \boldsymbol{v} dt + \frac{\partial L}{\partial \dot{\boldsymbol{q}}} \boldsymbol{v} \Big|_{t_0}^{t_1} \tag{1.2}$$

Problem 1.1. Show that the action functional is given by the evaluation of the 1-form Ldt on $TM \times \mathbb{R}$ over the 1-chain $\tilde{\gamma}$ on $TM \times \mathbb{R}$,

$$S(\gamma) = \int_{\tilde{\gamma}} Ldt,$$

where $\tilde{\gamma} = \{(\gamma'(t), t)\,; t_0 \le t \le t_1\}$ and $Ldt\left(w, c\frac{\partial}{\partial t}\right) = cL(q, v), w \in T_{(q,v)}TM, c \in \mathbb{R}$.

Problem 1.2. Let $f \in C^\infty(M)$. Show that Lagrangian systems (M, L) and $(M, L + df)$ (where df is a fibre-wise linear function on TM) have the same equations of motion.

Problem 1.3. Give examples of Lagrangian systems such that an extremal connecting two given points (i) is not a local minimum; (ii) is not unique; (iii) does not exist.

Problem 1.4. For γ an extremal of the action functional S, the second variation of S is defined by

$$\delta^2_{V_1 V_2} S = \frac{\partial^2}{\partial \varepsilon_1 \partial \varepsilon_2} \Big|_{\varepsilon_1 = \varepsilon_2 = 0} S\left(\gamma_{\varepsilon_1, \varepsilon_2}\right)$$

where $\gamma_{\varepsilon_1, \varepsilon_2}$ is a smooth two-parameter family of paths in M such that the paths $\gamma_{\varepsilon_1, 0}$ and $\gamma_{0, \varepsilon_2}$ in $P(M)$ at the point $\gamma_{0,0} = \gamma \in P(M)$ have tangent vectors V_1 and V_2, respectively. For a Lagrangian system (M, L) find the second variation of S and verify that for given V_1 and V_2 it does not depend on the choice of $\gamma_{\varepsilon_1, \varepsilon_2}$.

1.3. Examples of Lagrangian systems. To describe a mechanical phenomena it is necessary to choose a frame of reference. The properties of the space-time where the motion takes place depend on this choice. The space-time is characterized by the following postulates [7].

Newtonian Space-Time. The space is a three-dimensional affine Euclidean space E^3. A choice of the origin $0 \in E^3$ - a reference point establishes the isomorphism $E^3 \simeq \mathbb{R}^3$, where the vector space $\mathbb{R}^3$ carries the Euclidean inner product and has a fixed orientation. The time is onedimensional - a time axis $\mathbb{R}$ - and the space-time is a direct product $E^3 \times \mathbb{R}$. An inertial reference frame is a coordinate system with respect to the origin $0 \in E^3$, initial time t_0, and an orthonormal basis in $\mathbb{R}^3$. In an inertial frame the space is homogeneous and isotropic and the time is homogeneous. The laws of motion are invariant with respect to the transformations

$$\boldsymbol{r} \mapsto g \cdot \boldsymbol{r} + \boldsymbol{r}_0, \quad t \mapsto t + t_0,$$

where $r, r_0 \in \mathbb{R}^3$ and g is an orthogonal linear transformation in $\mathbb{R}^3$. The time in classical mechanics is absolute.

The Galilean group is the group of all affine transformations of $E^3 \times \mathbb{R}$ which preserve time intervals and which for every $t \in \mathbb{R}$ are isometries in E^3. Every Galilean transformation is a composition of rotation, space-time translation, and a transformation

[7] Strictly speaking, these postulates are valid only in the non-relativistic limit of special relativity, when the speed of light in the vacuum is assumed to be infinite.

$$\boldsymbol{r} \mapsto \boldsymbol{r} + \boldsymbol{v}t, \quad t \mapsto t$$

where $v \in \mathbb{R}^3$. Any two inertial frames are related by a Galilean transformation.

Galileo's Relativity Principle. The laws of motion are invariant with respect to the Galilean group.

These postulates impose restrictions on Lagrangians of mechanical systems. Thus it follows from the first postulate that the Lagrangian L of a closed system does not explicitly depend on time. Physical systems are described by special Lagrangians, in agreement with the experimental facts about the motion of material bodies.

Example 1.1 (Free particle). The configuration space for a free particle is $M = \mathbb{R}^3$, and it can be deduced from Galileo's relativity principle that the Lagrangian for a free particle is

$$L = \frac{1}{2} m \dot{\boldsymbol{r}}^2.$$

Here $m > 0$[08] is the mass of a particle and $\dot{\boldsymbol{r}}^2 = |\dot{\boldsymbol{r}}|^2$ is the length square of the velocity vector $\dot{\boldsymbol{r}} \in T_{\boldsymbol{r}}\mathbb{R}^3 \simeq \mathbb{R}^3$. Euler-Lagrange equations give Newton's law of inertia,

$$\ddot{\boldsymbol{r}} = 0.$$

Example 1.2 (Interacting particles). A closed system of N interacting particles in $\mathbb{R}^3$ with masses $m_1, ..., m_N$ is described by a configuration space

$$M = \mathbb{R}^{3N} = \underbrace{\mathbb{R}^3 \times \cdots \times \mathbb{R}^3}_{N}$$

with a position vector $\boldsymbol{r} = (\boldsymbol{r}_1, ..., \boldsymbol{r}_N)$, where $\boldsymbol{r}_a \in \mathbb{R}^3$ is the position vector of the a-th particle, $a = 1, ..., N$. It is found that the Lagrangian is given by

$$L = \sum_{a=1}^{N} \frac{1}{2} m_a \dot{\boldsymbol{r}}_a^2 - V(\boldsymbol{r}) = T - V,$$

where

$$T = \sum_{a=1}^{N} \frac{1}{2} m_a \dot{\boldsymbol{r}}_a^2$$

is called kinetic energy of a system and $V(\boldsymbol{r})$ is potential energy. The Euler-Lagrange equations give Newton's equations

$$m_a \ddot{\boldsymbol{r}}_a = \boldsymbol{F}_a$$

where

$$\boldsymbol{F}_a = -\frac{\partial V}{\partial \boldsymbol{r}_a}$$

is the force on the a-th particle, $a = 1, ..., N$. Forces of this form are called conservative. It follows from homogeneity of space that potential energy $V(\boldsymbol{r})$ of a closed system of N interacting particles with conservative forces depends only on relative positions of the particles, which leads to the equation

[08] Otherwise the action functional is not bounded from below.

$$\sum_{a=1}^{N} \boldsymbol{F}_a = 0$$

In particular, for a closed system of two particles $\boldsymbol{F}_1 + \boldsymbol{F}_2 = 0$, which is the equality of action and reaction forces, also called Newton's third law.

The potential energy of a closed system with only pair-wise interaction between the particles has the form

$$V(\boldsymbol{r}) = \sum_{1 \le a < b \le N} V_{ab}\left(\boldsymbol{r}_a - \boldsymbol{r}_b\right)$$

It follows from the isotropy of space that $V(\boldsymbol{r})$ depends only on relative distances between the particles, so that the Lagrangian of a closed system of N particles with pair-wise interaction has the form

$$L = \sum_{a=1}^{N} \frac{1}{2} m_a \dot{\boldsymbol{r}}_a^2 - \sum_{1 \le a < b \le N} V_{ab}\left(|\boldsymbol{r}_a - \boldsymbol{r}_b|\right)$$

If the potential energy $V(\boldsymbol{r})$ is a homogeneous function of degree ρ, $V(\lambda \boldsymbol{r}) = \lambda^\rho V(\boldsymbol{r})$, then the average values $\bar{T}$ and $\bar{V}$ of kinetic energy and potential energy over a closed trajectory are related by the virial theorem

$$2\bar{T} = \rho \bar{V} \tag{1.3}$$

Indeed, let $\boldsymbol{r}(t)$ be a periodic trajectory with period $\tau > 0$, i.e., $\boldsymbol{r}(0) = \boldsymbol{r}(\tau)$, $\dot{\boldsymbol{r}}(0) = \dot{\boldsymbol{r}}(\tau)$. Using integration by parts, Newton's equations, and Euler's homogeneous function theorem, we get

$$\begin{aligned} 2\bar{T} &= \frac{1}{\tau} \int_0^\tau \sum_{a=1}^{N} m_a \dot{\boldsymbol{r}}_a^2 dt = -\frac{1}{\tau} \int_0^\tau \sum_{a=1}^{N} m_a \boldsymbol{r}_a \ddot{\boldsymbol{r}}_a dt \\ &= \frac{1}{\tau} \int_0^\tau \sum_{a=1}^{N} \boldsymbol{r}_a \frac{\partial V}{\partial \boldsymbol{r}_a} dt = \rho \bar{V} \end{aligned}$$

Example 1.3 (Universal gravitation). According to Newton's law of gravitation, the potential energy of the gravitational force between two particles with masses m_a and m_b is

$$V\left(\boldsymbol{r}_a - \boldsymbol{r}_b\right) = -G \frac{m_a m_b}{|\boldsymbol{r}_a - \boldsymbol{r}_b|},$$

where G is the gravitational constant. The configuration space of N particles with gravitational interaction is

$$M = \left\{ (\boldsymbol{r}_1, ..., \boldsymbol{r}_N) \in \mathbb{R}^{3N} : \boldsymbol{r}_a \neq \boldsymbol{r}_b \text{ for } a \neq b, a, b = 1, ..., N \right\}$$

Example 1.4 (Particle in an external potential field). Here $M = \mathbb{R}^3$ and

$$L = \frac{1}{2} m \dot{\boldsymbol{r}}^2 - V(\boldsymbol{r}, t)$$

where potential energy can explicitly depend on time. Equations of motion are Newton's equations

$$m \ddot{\boldsymbol{r}} = \boldsymbol{F} = -\frac{\partial V}{\partial \boldsymbol{r}}.$$

If $V = V(|\boldsymbol{r}|)$ is a function only of the distance $|\boldsymbol{r}|$, the potential field is called central.

Example 1.5 (Charged particle in electromagnetic field [9]). Consider a particle of charge e and mass m in $\mathbb{R}^3$ moving in a time-independent electromagnetic field with scalar and vector potentials $\varphi(\boldsymbol{r})$ and $\boldsymbol{A}(\boldsymbol{r}) = (A_1(\boldsymbol{r}), A_2(\boldsymbol{r}), A_3(\boldsymbol{r}))$. The Lagrangian has the form

$$L = \frac{m\dot{\boldsymbol{r}}^2}{2} + e\left(\frac{\dot{\boldsymbol{r}}\boldsymbol{A}}{c} - \varphi\right),$$

where c is the speed of light. The Euler-Lagrange equations give Newton's equations with the Lorentz force,

$$m\ddot{\boldsymbol{r}} = e\left(\boldsymbol{E} + \frac{\dot{\boldsymbol{r}}}{c} \times \boldsymbol{B}\right)$$

where $\times$ is the cross-product of vectors in $\mathbb{R}^3$, and

$$\boldsymbol{E} = -\frac{\partial\varphi}{\partial\boldsymbol{r}} \quad \text{and} \quad \boldsymbol{B} = \operatorname{curl}\boldsymbol{A}$$

are electric and magnetic [10] fields, respectively.

Example 1.6 (Small oscillations). Consider a particle of mass m with n degrees of freedom moving in a potential field $V(\boldsymbol{q})$, and suppose that potential energy U has a minimum at $\boldsymbol{q} = 0$. Expanding $V(\boldsymbol{q})$ in Taylor series around 0 and keeping only quadratic terms, one obtains a Lagrangian system which describes small oscillations from equilibrium. Explicitly,

$$L = \frac{1}{2}m\dot{\boldsymbol{q}}^2 - V_0(\boldsymbol{q}),$$

where V_0 is a positive-definite quadratic form on $\mathbb{R}^n$ given by

$$V_0(\boldsymbol{q}) = \frac{1}{2}\sum_{i,j=1}^{n}\frac{\partial^2 V}{\partial q^i \partial q^j}(0)q^i q^j$$

Since every quadratic form can be diagonalized by an orthogonal transformation, we can assume from the very beginning that coordinates $\boldsymbol{q} = (q^1, \ldots, q^n)$ are chosen so that $V_0(\boldsymbol{q})$ is diagonal and

$$L = \frac{1}{2}m\left(\dot{\boldsymbol{q}}^2 - \sum_{i=1}^{n}\omega_i^2\left(q^i\right)^2\right) \tag{1.4}$$

where $\omega_1, \ldots, \omega_n > 0$. Such coordinates $\boldsymbol{q}$ are called normal coordinates. In normal coordinates Euler-Lagrange equations take the form

$$\ddot{q}^i + \omega_i^2 q^i = 0, \quad i = 1, \ldots, n$$

and describe n decoupled (i.e., non-interacting) harmonic oscillators with frequencies $\omega_1, \ldots, \omega_n$.

Example 1.7 (Free particle on a Riemannian manifold). Let (M, ds^2) be a Riemannian manifold with the Riemannian metric ds^2. In local coordinates $x^1, \ldots, x^n$ on M,

$$ds^2 = g_{\mu\nu}(x)dx^\mu dx^\nu$$

where following tradition we assume the summation over repeated indices. The Lagrangian of a free particle on M is

[09] This is a non-relativistic limit of an example in classical electrodynamics.

$$L(v) = \frac{1}{2}\langle v, v\rangle = \frac{1}{2}\|v\|^2, v \in TM,$$

[10] Notation $\boldsymbol{B} = \text{rot}\,\boldsymbol{A}$ is also used.

where $\langle,\rangle$ stands for the inner product in fibers of TM given by the Riemannian metric. The corresponding functional

$$S(\gamma) = \frac{1}{2}\int_{t_0}^{t_1} \|\gamma'(t)\|^2\, dt = \frac{1}{2}\int_{t_0}^{t_1} g_{\mu\nu}(x)\dot{x}^\mu\dot{x}^\nu dt$$

is called the action functional in Riemannian geometry. The Euler-Lagrange equations are

$$g_{\mu\nu}\ddot{x}^\mu + \frac{\partial g_{\mu\nu}}{\partial x^\lambda}\dot{x}^\mu\dot{x}^\lambda = \frac{1}{2}\frac{\partial g_{\mu\lambda}}{\partial x^\nu}\dot{x}^\mu\dot{x}^\lambda,$$

and after multiplying by the inverse metric tensor $g^{\sigma\nu}$ and summation over ν they take the form

$$\ddot{x}^\sigma + \Gamma^\sigma_{\mu\nu}\dot{x}^\mu\dot{x}^\nu = 0, \quad \sigma = 1, ..., n,$$

where

$$\Gamma^\sigma_{\mu\nu} = \frac{1}{2}g^{\sigma\lambda}\left(\frac{\partial g_{\mu\lambda}}{\partial x^\nu} + \frac{\partial g_{\nu\lambda}}{\partial x^\mu} - \frac{\partial g_{\mu\nu}}{\partial x^\lambda}\right)$$

are Christoffel's symbols. The Euler-Lagrange equations of a free particle moving on a Riemannian manifold are geodesic equations.

Let ∇ be the Levi-Civita connection - the metric connection in the tangent bundle TM - and let ∇_ξ be a covariant derivative with respect to the vector field $\xi \in \text{Vect}(M)$. Explicitly,

$$(\nabla_\xi\eta)^\mu = \left(\frac{\partial\eta^\mu}{\partial x^\nu} + \Gamma^\mu_{\nu\lambda}\eta^\lambda\right)\xi^\nu, \quad \text{where} \quad \xi = \xi^\mu(x)\frac{\partial}{\partial x^\mu}, \eta = \eta^\mu(x)\frac{\partial}{\partial x^\mu}$$

For a path $\gamma(t) = (x^\mu(t))$ denote by $\nabla_{\dot\gamma}$ a covariant derivative along γ,

$$(\nabla_{\dot\gamma}\eta)^\mu(t) = \frac{d\eta^\mu(t)}{dt} + \Gamma^\mu_{\nu\lambda}(\gamma(t))\dot{x}^\nu(t)\eta^\lambda(t), \quad \text{where} \quad \eta = \eta^\mu(t)\frac{\partial}{\partial x^\mu}$$

is a vector field along γ. Formula (1.1) can now be written in an invariant form

$$\delta S = -\int_{t_0}^{t_1} \langle\nabla_{\dot\gamma}\dot\gamma, \delta\gamma\rangle\, dt$$

which is known as the formula for the first variation of the action in Riemannian geometry.

Example 1.8 (The rigid body). The configuration space of a rigid body in $\mathbb{R}^3$ with a fixed point is a Lie group $G = \text{SO}(3)$ of orientation preserving orthogonal linear transformations in $\mathbb{R}^3$. Every left-invariant Riemannian metric $\langle,\rangle onG$ defines a Lagrangian $L : TG \to \mathbb{R}$ by

$$L(v) = \frac{1}{2}\langle v, v\rangle, \quad v \in TG.$$

According to the previous example, equations of motion of a rigid body are geodesic equations on G with respect to the Riemannian metric $\langle,\rangle.Let\ \mathfrak{g} = \mathfrak{so}(3)$ be the Lie algebra of G. A velocity vector $\dot g \in T_gG$ defines the angular velocity of the body by $\Omega = (L_{g^{-1}})_*\,\dot g \in \mathfrak{g}$, where $L_g : G \to G$ are left translations on G. In terms of angular velocity, the Lagrangian takes the form

$$L = \frac{1}{2}\langle\Omega, \Omega\rangle_e$$

where $\langle , \rangle_e$ is an inner product on $\mathfrak{g} = T_eG$ given by the Riemannian metric $\langle , \rangle$. The Lie algebra $\mathfrak{g}$ - the Lie algebra of 3×3 skew-symmetric matrices has the invariant inner product $\langle u, v \rangle_0 = -\frac{1}{2} \operatorname{Tr} uv$ (the Killing form), so that $\langle \Omega, \Omega \rangle_e = \langle \boldsymbol{A} \cdot \Omega, \Omega \rangle_0$ for some symmetric linear operator $\boldsymbol{A} : \mathfrak{g} \to \mathfrak{g}$ which is positive-definite with respect to the Killing form. Such a linear operator $\boldsymbol{A}$ is called the inertia tensor of the body. The principal axes of inertia of the body are orthonormal eigenvectors e_1, e_2, e_3 of $\boldsymbol{A}$; corresponding eigenvalues I_1, I_2, I_3 are called the principal moments of inertia. Setting $\Omega = \Omega_1 e_1 + \Omega_2 e_2 + \Omega_3 e_3$[11], we get

$$L = \frac{1}{2} \left(I_1 \Omega_1^2 + I_2 \Omega_2^2 + I_3 \Omega_3^2 \right).$$

In this parametrization, the Euler-Lagrange equations become Euler's equations

$$\begin{aligned} I_1 \dot{\Omega}_1 &= (I_2 - I_3)\, \Omega_2 \Omega_3 \\ I_2 \dot{\Omega}_2 &= (I_3 - I_1)\, \Omega_1 \Omega_3 \\ I_3 \dot{\Omega}_3 &= (I_1 - I_2)\, \Omega_1 \Omega_2 \end{aligned}$$

Euler's equations describe the rotation of a free rigid body around a fixed point. In the system of coordinates with axes which are the principal axes of inertia, principal moments of inertia of the body are I_1, I_2, I_3.

Problem 1.5. Determine the motion of a charged particle in a constant uniform magnetic field. Show that if the initial velocity $v_3 = 0$ in the z-axis (taken in the direction of the field, $\boldsymbol{B} = (0, 0, B)$), the trajectories are circles of radii $r = \frac{cmv_t}{eB}$ in a plane perpendicular to the field (the xy-plane), where $v_t = \sqrt{v_1^2 + v_2^2}$ is the initial velocity in the xy-plane. The centers (x_0, y_0) of circles are given by

$$x_0 = \frac{cmv_1}{eB} + x, \quad y_0 = -\frac{cmv_2}{eB} + y$$

where (x, y) are points on a circle of radius r.

Problem 1.6. Show that the Euler-Lagrange equations for the Lagrangian $L(v) = \|v\|, v \in TM$, coincide with the geodesic equations written with respect to a constant multiple of the natural parameter.

Problem 1.7. Prove that for a particle in a potential field, discussed in Example 1.4, the second variation of the action functional, defined in Problem 1.4, is given by

$$\delta^2 S = \int_{t_0}^{t_1} \mathcal{J}\left(\delta_1 \boldsymbol{r}\right) \delta_2 \boldsymbol{r} dt$$

[11] This establishes the Lie algebra isomorphism $\mathfrak{g} \simeq \mathbb{R}^3$, where the Lie bracket in $\mathbb{R}^3$ is given by the cross-product.

where $\delta_1 \boldsymbol{r}, \delta_2 \boldsymbol{r} \in T_\gamma P\mathbb{R}^3, \gamma = \boldsymbol{r}(t)$ is the classical trajectory, $\mathcal{J} = -m\frac{d^2}{dt^2} I - \frac{\partial^2 V}{\partial \boldsymbol{r}^2}(t)$, I is the 3×3 identity matrix, and $\frac{\partial^2 V}{\partial \boldsymbol{r}^2}(t) = \left\{ \frac{\partial^2 V}{\partial \boldsymbol{r}_a \partial \boldsymbol{r}_b}(\boldsymbol{r}(t)) \right\}_{a,b=1}^{3}$. A second-order linear differential operator $\mathcal{J}$, acting on vector fields along γ, is called the Jacobi operator.

Problem 1.8. Find normal coordinates and frequencies for the Lagrangian system considered in Example 1.6 with $V_0(\boldsymbol{q}) = \frac{1}{2} a^2 \sum_{i=1}^{n} \left(q^{i+1} - q^i\right)^2$, where $q^{n+1} = q^1$.

Problem 1.9. Prove that the second variation of the action functional in Riemannian geometry is given by

$$\delta^2 S = \int_{t_0}^{t_1} \langle \mathcal{J}(\delta_1\gamma), \delta_2\gamma \rangle \, dt$$

Here $\delta_1\gamma, \delta_2\gamma \in T_\gamma PM$, $\mathcal{J} = -\nabla_{\dot\gamma}^2 - R(\dot\gamma, \cdot)\dot\gamma$ is the Jacobi operator, and R is a curvature operator - a fibre-wise linear mapping $R : TM \otimes TM \to \mathrm{End}(TM)$ of vector bundles, defined by $R(\xi,\eta) = \nabla_\eta\nabla_\xi - \nabla_\xi\nabla_\eta + \nabla_{[\xi,\eta]} : TM \to TM$, where $\xi, \eta \in \mathrm{Vect}(M)$.

Problem 1.10. Choosing the principal axes of inertia as a basis in $\mathbb{R}^3$, show that the Lie algebra isomorphism $\mathfrak{g} \simeq \mathbb{R}^3$ is given by $\mathfrak{g} \ni \begin{pmatrix} 0 & -\Omega_3 & \Omega_2 \\ \Omega_3 & 0 & \\ -\Omega_2 & \Omega_1 & -\Omega_1 \end{pmatrix} \mapsto (\Omega_1, \Omega_2, \Omega_3) \in \mathbb{R}^3$.

Problem 1.11. Show that for every symmetric $\boldsymbol{A} \in \mathrm{End}\ \mathfrak{g}$ there exists a symmetric 3×3 matrix A such that $\boldsymbol{A} \cdot \Omega = A\Omega + \Omega A$, and find A for diagonal $\boldsymbol{A}$.

Problem 1.12. Derive Euler's equations for a rigid body. (Hint: Use that $L = -\frac{1}{2}\,\mathrm{Tr}\, A\Omega^2$, where $\Omega = g^{-1}\dot g$ and $\delta\Omega = -g^{-1}\delta g\Omega + g^{-1}\delta\dot g$, and obtain the EulerLagrange equations in the matrix form $A\dot\Omega + \dot\Omega A = A\Omega^2 - \Omega^2 A$.)

1.4. Symmetries and Noether's theorem.

To describe the motion of a mechanical system one needs to solve the corresponding Euler-Lagrange equations - a system of second order ordinary differential equations for the generalized coordinates. This could be a very difficult problem. Therefore of particular interest are those functions of generalized coordinates and velocities which remain constant during the motion.

Definition. A smooth function $I : TM \to \mathbb{R}$ is called the integral of motion (first integral, or conservation law) for a Lagrangian system (M, L) if

$$\frac{d}{dt} I(\gamma'(t)) = 0$$

for all extremals γ of the action functional.

Definition. The energy of a Lagrangian system (M, L) is a function E on $TM \times \mathbb{R}$ defined in standard coordinates on TM by

$$E(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) = \sum_{i=1}^{n} \dot q^i \frac{\partial L}{\partial \dot q^i}(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) - L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)$$

Lemma 1.1. The energy $E = \dot{\boldsymbol{q}}\frac{\partial L}{\partial \dot{\boldsymbol{q}}} - L$ is a well-defined function on $TM \times \mathbb{R}$.

Proof. Let (U, φ) and (U', φ') be coordinate charts on M with the transition functions $F = (F^1, ..., F^n) = \varphi' \circ \varphi^{-1} : \varphi(U \cap U') \to \varphi'(U \cap U')$. Corresponding standard coordinates $(\boldsymbol{q}, \dot{\boldsymbol{q}})$ and $(\boldsymbol{q}', \dot{\boldsymbol{q}}')$ are related by $\boldsymbol{q}' = F(\boldsymbol{q})$ and $\dot{\boldsymbol{q}}' = F_*(\boldsymbol{q})\dot{\boldsymbol{q}}$ (see Section 1.2). We have $d\boldsymbol{q}' = F_*(\boldsymbol{q})d\boldsymbol{q}$ and $d\dot{\boldsymbol{q}}' = G(\boldsymbol{q}, \dot{\boldsymbol{q}})d\boldsymbol{q} + F_*(\boldsymbol{q})d\dot{\boldsymbol{q}}$ (for some matrix-valued function $G(\boldsymbol{q}, \dot{\boldsymbol{q}})$), so that

$$\begin{aligned} dL &= \frac{\partial L}{\partial \boldsymbol{q}'} d\boldsymbol{q}' + \frac{\partial L}{\partial \dot{\boldsymbol{q}}'} d\dot{\boldsymbol{q}}' + \frac{\partial L}{\partial t} dt \\ &= \left(\frac{\partial L}{\partial \boldsymbol{q}'} F_*(\boldsymbol{q}) + \frac{\partial L}{\partial \dot{\boldsymbol{q}}'} G(\boldsymbol{q}, \dot{\boldsymbol{q}}) \right) d\boldsymbol{q} + \frac{\partial L}{\partial \dot{\boldsymbol{q}}'} F_*(\boldsymbol{q}) d\dot{\boldsymbol{q}} + \frac{\partial L}{\partial t} dt \\ &= \frac{\partial L}{\partial \boldsymbol{q}} d\boldsymbol{q} + \frac{\partial L}{\partial \dot{\boldsymbol{q}}} d\dot{\boldsymbol{q}} + \frac{\partial L}{\partial t} dt. \end{aligned}$$

Thus under a change of coordinates

$$\frac{\partial L}{\partial \dot{\boldsymbol{q}}'} F_*(\boldsymbol{q}) = \frac{\partial L}{\partial \dot{\boldsymbol{q}}} \quad \text{and} \quad \dot{\boldsymbol{q}}' \frac{\partial L}{\partial \dot{\boldsymbol{q}}'} = \dot{\boldsymbol{q}} \frac{\partial L}{\partial \dot{\boldsymbol{q}}},$$

so that E is a well-defined function on TM.

Corollary 1.2. Under a change of local coordinates on M, components of $\frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) = \left(\frac{\partial L}{\partial \dot{q}^1}, ..., \frac{\partial L}{\partial \dot{q}^n} \right)$ transform like components of a 1-form on M.

Proposition 1.1 (Conservation of energy). The energy of a closed system is an integral of motion.

Proof. For an extremal γ set $E(t) = E(\gamma(t))$. We have, according to the Euler-Lagrange equations,

$$\begin{aligned} \frac{dE}{dt} &= \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\boldsymbol{q}}} \right) \dot{\boldsymbol{q}} + \frac{\partial L}{\partial \dot{\boldsymbol{q}}} \ddot{\boldsymbol{q}} - \frac{\partial L}{\partial \boldsymbol{q}} \dot{\boldsymbol{q}} - \frac{\partial L}{\partial \dot{\boldsymbol{q}}} \ddot{\boldsymbol{q}} - \frac{\partial L}{\partial t} \\ &= \left(\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\boldsymbol{q}}} \right) - \frac{\partial L}{\partial \boldsymbol{q}} \right) \dot{\boldsymbol{q}} - \frac{\partial L}{\partial t} = -\frac{\partial L}{\partial t} \end{aligned}$$

Since for a closed system $\frac{\partial L}{\partial t} = 0$, the energy is conserved.

Conservation of energy for a closed mechanical system is a fundamental law of physics which follows from the homogeneity of time. For a general closed system of N interacting particles considered in Example 1.2,

$$E = \sum_{a=1}^{N} m_a \dot{\boldsymbol{r}}_a^2 - L = \sum_{a=1}^{N} \frac{1}{2} m_a \dot{\boldsymbol{r}}_a^2 + V(\boldsymbol{r}).$$

In other words, the total energy $E = T + V$ is a sum of the kinetic energy and the potential energy.

Definition. A Lagrangian $L : TM \to \mathbb{R}$ is invariant with respect to the diffeomorphism $g : M \to M$ if $L(g_*(v)) = L(v)$ for all $v \in TM$. The diffeomorphism g is called the symmetry of a closed Lagrangian system (M, L). A Lie group G is the symmetry group of (M, L) (group of continuous symmetries) if there is a left G-action on M such that for every $g \in G$ the mapping $M \ni x \mapsto g \cdot x \in M$ is a symmetry.

Continuous symmetries give rise to conservation laws.

Theorem 1.3 (Noether). Suppose that a Lagrangian $L : TM \to \mathbb{R}$ is invariant under a one-parameter group $\{g_s\}_{s \in \mathbb{R}}$ of diffeomorphisms of M. Then the Lagrangian system (M, L) admits an integral of motion I, given in standard coordinates on TM by

$$I(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}^i}(\boldsymbol{q}, \dot{\boldsymbol{q}}) \left(\left. \frac{dg_s^i(\boldsymbol{q})}{ds} \right|_{s=0} \right) = \frac{\partial L}{\partial \dot{\boldsymbol{q}}} \boldsymbol{a}$$

where $X = \sum_{i=1}^{n} a^i(\boldsymbol{q}) \frac{\partial}{\partial q^i}$ is the vector field on M associated with the flow g_s. The integral of motion I is called the Noether integral.

Proof. It follows from Corollary 1.2 that I is a well-defined function on TM. Now differentiating $L\left(\left(g_s\right)_*\left(\gamma'(t)\right)\right) = L\left(\gamma'(t)\right)$ with respect to s at $s = 0$ and using the Euler-Lagrange equations we get

$$0 = \frac{\partial L}{\partial \boldsymbol{q}}\boldsymbol{a} + \frac{\partial L}{\partial \dot{\boldsymbol{q}}}\dot{\boldsymbol{a}} = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\boldsymbol{q}}}\right)\boldsymbol{a} + \frac{\partial L}{\partial \dot{\boldsymbol{q}}}\frac{d\boldsymbol{a}}{dt} = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\boldsymbol{q}}}\boldsymbol{a}\right),$$

where $\boldsymbol{a}(t) = (a^1(\gamma(t)), ..., a^n(\gamma(t)))$.

Remark. A vector field X on M is called an infinitesimal symmetry if the corresponding local flow g_s of X (defined for each $s \in \mathbb{R}$ on some $U_s \subseteq M$) is a symmetry: $L \circ \left(g_s\right)_* = L$ on U_s. Every vector field X on M lifts to a vector field X' on TM, defined by a local flow on TM induced from the corresponding local flow on M. In standard coordinates on TM,

$$X = \sum_{i=1}^{n} a^i(\boldsymbol{q})\frac{\partial}{\partial q^i} \quad \text{and} \quad X' = \sum_{i=1}^{n} a^i(\boldsymbol{q})\frac{\partial}{\partial q^i} + \sum_{i,j=1}^{n} \dot{q}^j \frac{\partial a^i}{\partial q^j}(\boldsymbol{q})\frac{\partial}{\partial \dot{q}^i}. \tag{1.5}$$

It is easy to verify that X is an infinitesimal symmetry if and only if $dL\left(X'\right) = 0$ on TM, which in standard coordinates has the form

$$\sum_{i=1}^{n} a^i(\boldsymbol{q})\frac{\partial L}{\partial q^i} + \sum_{i,j=1}^{n} \dot{q}^j \frac{\partial a^i}{\partial q^j}(\boldsymbol{q})\frac{\partial L}{\partial \dot{q}^i} = 0. \tag{1.6}$$

Remark. Noether's theorem generalizes to time-dependent Lagrangians L: $TM \times \mathbb{R} \to \mathbb{R}$. Namely, on the extended configuration space $M_1 = M \times \mathbb{R}$ define a time-independent Lagrangian L_1 by

$$L_1(\boldsymbol{q}, \tau, \dot{\boldsymbol{q}}, \dot{\tau}) = L\left(\boldsymbol{q}, \frac{\dot{\boldsymbol{q}}}{\dot{\tau}}, \tau\right)\dot{\tau}$$

where $(\boldsymbol{q}, \tau)$ are local coordinates on M_1 and $(\boldsymbol{q}, \tau, \dot{\boldsymbol{q}}, \dot{\tau})$ are standard coordinates on TM_1. The Noether integral I_1 for a closed system (M_1, L_1) defines an integral of motion I for a system (M, L) by the formula

$$I(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) = I_1(\boldsymbol{q}, t, \dot{\boldsymbol{q}}, 1).$$

When the Lagrangian L does not depend on time, L_1 is invariant with respect to the one-parameter group of translations $\tau \mapsto \tau + s$, and the Noether integral $I_1 = \frac{\partial L_1}{\partial \dot{\tau}}$ gives $I = -E$.

Noether's theorem can be generalized as follows.

Proposition 1.2. Suppose that for the Lagrangian $L : TM \to \mathbb{R}$ there exist a vector field X on M and a function K on TM such that for every path γ in M,

$$dL\left(X'\right)\left(\gamma(t)\right) = \frac{d}{dt}K\left(\gamma'(t)\right)$$

Then

$$I = \sum_{i=1}^{n} a^i(\boldsymbol{q})\frac{\partial L}{\partial \dot{q}^i}(\boldsymbol{q}, \dot{\boldsymbol{q}}) - K(\boldsymbol{q}, \dot{\boldsymbol{q}})$$

is an integral of motion for the Lagrangian system (M, L).

Proof. Using Euler-Lagrange equations, we have along the extremal γ,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\boldsymbol{q}}}\boldsymbol{a}\right) = \frac{\partial L}{\partial \boldsymbol{q}}\boldsymbol{a} + \frac{\partial L}{\partial \dot{\boldsymbol{q}}}\dot{\boldsymbol{a}} = \frac{dK}{dt}.$$

Example 1.9 (Conservation of momentum). Let $M = V$ be a vector space, and suppose that a Lagrangian L is invariant with respect to a one-parameter group $g_s(q) = q + sv, v \in V$. According to Noether's theorem,

$$I = \sum_{i=1}^{n} v^i \frac{\partial L}{\partial \dot{q}^i}$$

is an integral of motion. Now let (M, L) be a closed Lagrangian system of N interacting particles considered in Example 1.2. We have $M = V = \mathbb{R}^{3N}$, and the Lagrangian L is invariant under simultaneous translation of
coordinates $\boldsymbol{r}_a = (r_a^1, r_a^2, r_a^3)$ of all particles by the same vector $\boldsymbol{c} \in \mathbb{R}^3$. Thus $v = (c, ..., c) \in \mathbb{R}^{3N}$ and for every $c = (c^1, c^2, c^3) \in \mathbb{R}^3$,

$$I = \sum_{a=1}^{N} \left(c^1 \frac{\partial L}{\partial \dot{r}_a^1} + c^2 \frac{\partial L}{\partial \dot{r}_a^2} + c^3 \frac{\partial L}{\partial \dot{r}_a^3} \right) = c^1 P_1 + c^2 P_2 + c^3 P_3$$

is an integral of motion. The integrals of motion P_1, P_2, P_3 define the vector

$$\boldsymbol{P} = \sum_{a=1}^{N} \frac{\partial L}{\partial \dot{\boldsymbol{r}}_a} \in \mathbb{R}^3$$

(or rather a vector in the dual space to $\mathbb{R}^3$), called the momentum of the system. Explicitly,

$$\boldsymbol{P} = \sum_{a=1}^{N} m_a \dot{r}_a$$

so that the total momentum of a closed system is the sum of momenta of individual particles. Conservation of momentum is a fundamental physical law which reflects the homogeneity of space.

Traditionally, $p_i = \frac{\partial L}{\partial \dot{q}^i}$ are called generalized momenta corresponding to generalized coordinates q^i, and $F_i = \frac{\partial L}{\partial q^i}$ are called generalized forces. In these notations, the Euler-Lagrange equations have the same form

$$\dot{p} = F$$

as Newton's equations in Cartesian coordinates. Conservation of momentum implies Newton's third law.

Example 1.10 (Conservation of angular momentum). Let $M = V$ be a vector space with Euclidean inner product. Let $G = \mathrm{SO}(V)$ be the connected Lie group of automorphisms of V preserving the inner product, and let $\mathfrak{g} = \mathfrak{so}(V)$ be the Lie algebra of G. Suppose that a Lagrangian L is invariant with respect to the action of a one-parameter subgroup $g_s(q) = e^{sx} \cdot q$ of G on V, where $x \in \mathfrak{g}$ and e^x is the exponential map. According to Noether's theorem,

$$I = \sum_{i=1}^{n} (x \cdot q)^i \frac{\partial L}{\partial \dot{q}^i}$$

is an integral of motion. Now let (M, L) be a closed Lagrangian system of N interacting particles considered in Example 1.2. We have $M = V = \mathbb{R}^{3N}$, and the Lagrangian L is invariant under a simultaneous rotation of coordinates $\boldsymbol{r}_a$ of all particles by the same orthogonal transformation in $\mathbb{R}^3$.

Thus $x = (u, ..., u) \in \underbrace{\mathfrak{so}(3) \oplus \cdots \oplus \mathfrak{so}(3)}_{N}$, and for every $u \in \mathfrak{so}(3)$,

$$I = \sum_{a=1}^{N} \left((u \cdot \boldsymbol{r}_a)^1 \frac{\partial L}{\partial \dot{r}_a^1} + (u \cdot \boldsymbol{r}_a)^2 \frac{\partial L}{\partial \dot{r}_a^2} + (u \cdot \boldsymbol{r}_a)^3 \frac{\partial L}{\partial \dot{r}_a^3} \right)$$

is an integral of motion. Let $u = u^1 X_1 + u^2 X_2 + u^3 X_3$, where $X_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, X_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, X_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ is the basis in $\mathfrak{so}(3) \simeq \mathbb{R}^3$ corresponding to the rotations about the vectors e_1, e_2, e_3 of the standard orthonormal basis in $\mathbb{R}^3$ (see Problem 1.10). We get

$$I = u^1 M_1 + u^2 M_2 + u^3 M_3,$$

where $\boldsymbol{M} = (M_1, M_2, M_3) \in \mathbb{R}^3$ (or rather a vector in the dual space to $\mathfrak{so}(3)$) is given by

$$\boldsymbol{M} = \sum_{a=1}^{N} \boldsymbol{r}_a \times \frac{\partial L}{\partial \dot{\boldsymbol{r}}_a}$$

The vector $\boldsymbol{M}$ is called the angular momentum of the system. Explicitly,

$$\boldsymbol{M} = \sum_{a=1}^{N} \boldsymbol{r}_a \times m_a \dot{\boldsymbol{r}}_a$$

so that the total angular momentum of a closed system is the sum of angular momenta of individual particles. Conservation of angular momentum is a fundamental physical law which reflects the isotropy of space.

Problem 1.13. Find how total momentum and total angular momentum transform under the Galilean transformations.

1.5. One-dimensional motion.

The motion of systems with one degree of freedom is called one-dimensional. In terms of a Cartesian coordinate x on $M = \mathbb{R}$ the Lagrangian takes the form

$$L = \frac{1}{2} m \dot{x}^2 - V(x)$$

The conservation of energy

$$E = \frac{1}{2} m \dot{x}^2 + V(x)$$

allows us to solve the equation of motion in a closed form by separation of variables. We have

$$\frac{dx}{dt} = \sqrt{\frac{2}{m}(E - V(x))}$$

so that

$$t = \sqrt{\frac{m}{2}} \int \frac{dx}{\sqrt{E - V(x)}}$$

The inverse function $x(t)$ is a general solution of Newton's equation

$$m\ddot{x} = -\frac{dV}{dx}$$

with two arbitrary constants, the energy E and the constant of integration.
Since kinetic energy is non-negative, for a given value of E the actual motion takes place in the region of $\mathbb{R}$ where $V(x) \leq E$. The points where $V(x) = E$ are called turning points. The motion which is confined between two turning points is called finite. The finite motion is periodic - the particle oscillates between the turning points x_1 and x_2 with the period

$$T(E) = \sqrt{2m}\int_{x_1}^{x_2} \frac{dx}{\sqrt{E - V(x)}}$$

If the region $V(x) \leq E$ is unbounded, then the motion is called infinite and the particle eventually goes to infinity. The regions where $V(x) > E$ are forbidden.

On the phase plane with coordinates (x, y) Newton's equation reduces to the first order system

$$m\dot{x} = y, \quad \dot{y} = -\frac{dV}{dx}$$

Trajectories correspond to the phase curves $(x(t), y(t))$, which lie on the level sets

$$\frac{y^2}{2m} + V(x) = E$$

of the energy function. The points $(x_0, 0)$, where x_0 is a critical point of the potential energy $V(x)$, correspond to the equilibrium solutions. The local minima correspond to the stable solutions and local maxima correspond to the unstable solutions. For the values of E which do not correspond to the equilibrium solutions the level sets are smooth curves. These curves are closed if the motion is finite.

The simplest non-trivial one-dimensional system, besides the free particle, is the harmonic oscillator with $V(x) = \frac{1}{2}kx^2 (k > 0)$, considered in Example 1.6. The general solution of the equation of motion is

$$x(t) = A\cos(\omega t + \alpha),$$

where A is the amplitude, $\omega = \sqrt{\frac{k}{m}}$ is the frequency, and α is the phase of a simple harmonic motion with the period $T = \frac{2\pi}{\omega}$. The energy is $E = \frac{1}{2}m\omega^2 A^2$ and the motion is finite with the same period T for $E > 0$.

Problem 1.14. Show that for $V(x) = -x^4$ there are phase curves which do not exist for all times. Prove that if $V(x) \geq 0$ for all x, then all phase curves exist for all times.

Problem 1.15. The simple pendulum is a Lagrangian system with $M = S^1 = \mathbb{R}/2\pi\mathbb{Z}$ and $L = \frac{1}{2}\dot{\theta}^2 + \cos\theta$. Find the period T of the pendulum as a function of the amplitude of the oscillations.

Problem 1.16. Suppose that the potential energy $V(x)$ is even, $V(0) = 0$, and $V(x)$ is a one-to-one monotonically increasing function for $x \geq 0$. Prove that the inverse function $x(V)$ and the period $T(E)$ are related by the Abel transform

$$T(E) = 2\sqrt{2m}\int_0^E \frac{dx}{dV}\frac{dV}{\sqrt{E - V}} \quad \text{and} \quad x(V) = \frac{1}{2\pi\sqrt{2m}}\int_0^V \frac{T(E)dE}{\sqrt{V - E}}$$

1.6. The motion in a central field and the Kepler problem. The motion of a system of two interacting particles - the two-body problem - can also be solved completely. Namely, in this case (see Example 1.2) $M = \mathbb{R}^6$ and

$$L = \frac{m_1 \dot{\boldsymbol{r}}_1^2}{2} + \frac{m_2 \dot{\boldsymbol{r}}_2^2}{2} - V\left(|\boldsymbol{r}_1 - \boldsymbol{r}_2|\right)$$

Introducing on $\mathbb{R}^6$ new coordinates

$$\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2 \quad \text{and} \quad \boldsymbol{R} = \frac{m_1 \boldsymbol{r}_1 + m_2 \boldsymbol{r}_2}{m_1 + m_2}$$

we get

$$L = \frac{1}{2} m \dot{\boldsymbol{R}}^2 + \frac{1}{2} \mu \dot{\boldsymbol{r}}^2 - V(|\boldsymbol{r}|)$$

where $m = m_1 + m_2$ is the total mass and $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is the reduced mass of a two-body system. The Lagrangian L depends only on the velocity $\dot{\boldsymbol{R}}$ of the center of mass and not on its position $\boldsymbol{R}$. A generalized coordinate with this property is called cyclic. It follows from the Euler-Lagrange equations that generalized momentum corresponding to the cyclic coordinate is conserved. In our case it is a total momentum of the system,

$$\boldsymbol{P} = \frac{\partial L}{\partial \dot{\boldsymbol{R}}} = m \dot{\boldsymbol{R}}$$

so that the center of mass $\boldsymbol{R}$ moves uniformly. Thus in the frame of reference where $\boldsymbol{R} = 0$, the two-body problem reduces to the problem of a single particle of mass μ in the external central field $V(|\boldsymbol{r}|)$. In spherical coordinates in $\mathbb{R}^3$,

$$x = r \sin\vartheta \cos\varphi, y = r \sin\vartheta \sin\varphi, z = r \cos\vartheta$$

where $0 \leq \vartheta < \pi, 0 \leq \varphi < 2\pi$, its Lagrangian takes the form

$$L = \frac{1}{2} \mu \left(\dot{r}^2 + r^2 \dot{\vartheta}^2 + r^2 \sin^2\vartheta \dot{\varphi}^2 \right) - V(r)$$

It follows from the conservation of angular momentum $\boldsymbol{M} = \mu \boldsymbol{r} \times \dot{\boldsymbol{r}}$ that during motion the position vector r lies in the plane P orthogonal to M in $\mathbb{R}^3$. Introducing polar coordinates (r, χ) in the plane P we get $\dot{\chi}^2 = \dot{\vartheta}^2 + \sin^2\vartheta \dot{\varphi}^2$, so that

$$L = \frac{1}{2} \mu \left(\dot{r}^2 + r^2 \dot{\chi}^2 \right) - V(r)$$

The coordinate χ is cyclic and its generalized momentum $\mu r^2 \dot{\chi}$ coincides with $|\boldsymbol{M}|$ if $\dot{\chi} > 0$ and with $-|\boldsymbol{M}|$ if $\dot{\chi} < 0$. Denoting this quantity by M, we get the equation

$$\mu r^2 \dot{\chi} = M \tag{1.7}$$

which is equivalent to Kepler's second law [12]. Using (1.7) we get for the total energy

$$E = \frac{1}{2} \mu \left(\dot{r}^2 + r^2 \dot{\chi}^2 \right) + V(r) = \frac{1}{2} \mu \dot{r}^2 + V(r) + \frac{M^2}{2 \mu r^2} \tag{1.8}$$

Thus the radial motion reduces to a one-dimensional motion on the half-line $r > 0$ with the effective potential energy

$$V_{eff}(r) = V(r) + \frac{M^2}{2 \mu r^2}$$

where the second term is called the centrifugal energy. As in the previous section, the solution is given by

$$t = \sqrt{\frac{\mu}{2}} \int \frac{dr}{\sqrt{E - V_{eff}(r)}} \tag{1.9}$$

It follows from (1.7) that the angle χ is a monotonic function of t, given by another quadrature

$$\chi = \frac{M}{\sqrt{2\mu}} \int \frac{dr}{r^2\sqrt{E - V_{eff}(r)}} \tag{1.10}$$

yielding an equation of the trajectory in polar coordinates.
The set $V_{eff}(r) \leq E$ is a union of annuli $0 \leq r_{\min} \leq r \leq r_{\max} \leq \infty$, and the motion is finite if $0 < r_{\min} \leq r \leq r_{\max} < \infty$. Though for a finite motion $r(t)$ oscillates between $r_{\min}$ and $r_{\max}$, corresponding trajectories are not necessarily closed. The necessary and sufficient condition for a finite motion to have a closed trajectory is that the angle

$$\Delta\chi = \frac{M}{\sqrt{2\mu}} \int_{r_{\min}}^{r_{\max}} \frac{dr}{r^2\sqrt{E - V_{eff}(r)}}$$

is commensurable with 2π, i.e., $\Delta\chi = 2\pi\frac{m}{n}$ for some $m, n \in \mathbb{Z}$. If the angle $\Delta\chi$ is not commensurable with 2π, the orbit is everywhere dense in the annulus $r_{\min} \leq r \leq r_{\max}$. If

$$\lim_{r\to\infty} V_{eff}(r) = \lim_{r\to\infty} V(r) = V < \infty$$

the motion is infinite for $E > V$ - the particle goes to ∞ with finite velocity $\sqrt{\frac{2}{\mu}(E - V)}$.

A very important special case is when

$$V(r) = -\frac{\alpha}{r}.$$

It describes Newton's gravitational attraction ($\alpha > 0$) and Coulomb electrostatic interaction (either attractive or repulsive). First consider the case when $\alpha > 0$ - Kepler's problem. The effective potential energy is

$$V_{eff}(r) = -\frac{\alpha}{r} + \frac{M^2}{2\mu r^2}$$

and has the global minimum

$$V_0 = -\frac{\alpha^2\mu}{2M^2}$$

at $r_0 = \frac{M^2}{\alpha\mu}$. The motion is infinite for $E \geq 0$ and is finite for $V_0 \leq E < 0$. The explicit form of trajectories can be determined by an elementary integration in (1.10), which gives

$$\chi = \cos^{-1} \frac{\frac{M}{r} - \frac{M}{r_0}}{\sqrt{2\mu\,(E - V_0)}} + C.$$

Choosing a constant of integration $C = 0$ and introducing notation

$$p = r_0 \quad \text{and} \quad e = \sqrt{1 - \frac{E}{V_0}},$$

we get the equation of the orbit (trajectory)

[012] It is the statement that sectorial velocity of a particle in a central field is constant.

$$\frac{p}{r} = 1 + e\cos\chi. \tag{1.11}$$

This is the equation of a conic section with one focus at the origin. Quantity $2p$ is called the latus rectum of the orbit, and e is called the eccentricity. The choice $C = 0$ is such that the point with $\chi = 0$ is the point nearest to the origin (called the perihelion). When $V_0 \le E < 0$, the eccentricity $e < 1$ so that the orbit is the ellipse [13] with the major and minor semi-axes

$$a = \frac{p}{1-e^2} = \frac{\alpha}{2|E|}, \quad b = \frac{p}{\sqrt{1-e^2}} = \frac{|M|}{\sqrt{2\mu|E|}}. \tag{1.12}$$

Correspondingly, $r_{\min} = \frac{p}{1+e}, r_{\max} = \frac{p}{1-e}$, and the period T of elliptic orbit is given by

$$T = \pi\alpha\sqrt{\frac{\mu}{2|E|^3}}.$$

The last formula is Kepler's third law. When $E > 0$, the eccentricity $e > 1$ and the motion is infinite - the orbit is a hyperbola with the origin as

internal focus. When $E = 0$, the eccentricity $e = 1$ - the particle starts from rest at ∞ and the orbit is a parabola.

For the repulsive case $\alpha < 0$ the effective potential energy $V_{eff}(r)$ is always positive and decreases monotonically from ∞ to 0 . The motion is always infinite and the trajectories are hyperbolas (parabola if $E = 0$)

$$\frac{p}{r} = -1 + e\cos\chi$$

with

$$p = \frac{M^2}{\alpha\mu} \quad \text{and} \quad e = \sqrt{1 + \frac{2EM^2}{\mu\alpha^2}}.$$

Kepler's problem is very special: for every $\alpha \in \mathbb{R}$ the Lagrangian system on $\mathbb{R}^3$ with

$$L = \frac{1}{2}\mu\dot{\boldsymbol{r}}^2 + \frac{\alpha}{r} \tag{1.13}$$

has three extra integrals of motion W_1, W_2, W_3 in addition to the components of the angular momentum $\boldsymbol{M}$. The corresponding vector $\boldsymbol{W} = (W_1, W_2, W_3)$, called the Laplace-Runge-Lenz vector, is given by

$$\boldsymbol{W} = \dot{\boldsymbol{r}} \times \boldsymbol{M} - \frac{\alpha\boldsymbol{r}}{r}. \tag{1.14}$$

Indeed, using equations of motion $\mu\ddot{\boldsymbol{r}} = -\frac{\alpha r}{r^3}$ and conservation of the angular momentum $\boldsymbol{M} = \mu\boldsymbol{r} \times \dot{\boldsymbol{r}}$, we get

$$\begin{aligned}
\dot{\boldsymbol{W}} &= \mu\ddot{\boldsymbol{r}} \times (\boldsymbol{r} \times \dot{\boldsymbol{r}}) - \frac{\alpha\dot{\boldsymbol{r}}}{r} + \frac{\alpha(\dot{\boldsymbol{r}} \cdot \boldsymbol{r})\boldsymbol{r}}{r^3} \\
&= (\mu\ddot{\boldsymbol{r}} \cdot \dot{\boldsymbol{r}})\boldsymbol{r} - (\mu\ddot{\boldsymbol{r}} \cdot \boldsymbol{r})\dot{\boldsymbol{r}} - \frac{\alpha\dot{\boldsymbol{r}}}{r} + \frac{\alpha(\dot{\boldsymbol{r}} \cdot \boldsymbol{r})\boldsymbol{r}}{r^3} \\
&= 0.
\end{aligned}$$

Using $\mu(\dot{\boldsymbol{r}} \times \boldsymbol{M}) \cdot \boldsymbol{r} = \boldsymbol{M}^2$ and the identity $(\boldsymbol{a} \times \boldsymbol{b})^2 = \boldsymbol{a}^2\boldsymbol{b}^2 - (\boldsymbol{a} \cdot \boldsymbol{b})^2$, we get

[013] The statement that planets have elliptic orbits with a focus at the Sun is Kepler's first law.

$$W^2 = \alpha^2 + \frac{2M^2E}{\mu} \tag{1.15}$$

where

$$E = \frac{\boldsymbol{p}^2}{2\mu} - \frac{\alpha}{r}$$

is the energy corresponding to the Lagrangian (1.13). The fact that all orbits are conic sections follows from this extra symmetry of Kepler's problem.

Problem 1.17. Prove all the statements made in this section.

Problem 1.18. Show that if

$$\lim_{r\to 0} V_{eff}(r) = -\infty,$$

then there are orbits with $r_{\min} = 0$ - "fall" of the particle to the center.

Problem 1.19. Prove that all finite trajectories in the central field are closed only when

$$V(r) = kr^2, k > 0, \quad \text{and} \quad V(r) = -\frac{\alpha}{r}, \alpha > 0$$

Problem 1.20. Find parametric equations for orbits in Kepler's problem.

Problem 1.21. Prove that the Laplace-Runge-Lenz vector $\boldsymbol{W}$ points in the direction of the major axis of the orbit and that $|\boldsymbol{W}| = \alpha e$, where e is the eccentricity of the orbit.

Problem 1.22. Using the conservation of the Laplace-Runge-Lenz vector, prove that trajectories in Kepler's problem with $E < 0$ are ellipses. (Hint: Evaluate $\boldsymbol{W} \cdot \boldsymbol{r}$ and use the result of the previous problem.)

1.7. Legendre transform. The equations of motion of a Lagrangian system (M, L) in standard coordinates associated with a coordinate chart $U \subset M$ are the Euler-Lagrange equations. In expanded form, they are given by the following system of second order ordinary differential equations:

$$\begin{aligned}\frac{\partial L}{\partial q^i}(\boldsymbol{q}, \dot{\boldsymbol{q}}) &= \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}(\boldsymbol{q}, \dot{\boldsymbol{q}})\right) \\ &= \sum_{j=1}^{n}\left(\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}(\boldsymbol{q}, \dot{\boldsymbol{q}})\ddot{q}^j + \frac{\partial^2 L}{\partial \dot{q}^i \partial q^j}(\boldsymbol{q}, \dot{\boldsymbol{q}})\dot{q}^j\right), \quad i = 1, ..., n.\end{aligned}$$

In order for this system to be solvable for the highest derivatives for all initial conditions in TU, the symmetric $n \times n$ matrix

$$H_L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \left\{\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}(\boldsymbol{q}, \dot{\boldsymbol{q}})\right\}_{i,j=1}^{n}$$

should be invertible on TU.

Definition. A Lagrangian system (M, L) is called non-degenerate if for every coordinate chart U on M the matrix $H_L(\boldsymbol{q}, \dot{\boldsymbol{q}})$ is invertible on TU.

Remark. Note that the $n \times n$ matrix H_L is a Hessian of the Lagrangian function L for vertical directions on TM. Under the change of standard coordinates $\boldsymbol{q}' = F(\boldsymbol{q})$ and $\boldsymbol{q}' = F_*(\boldsymbol{q})\boldsymbol{v}$ (see Section 1.2) it has the transformation law

$$H_L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = F_*(\boldsymbol{q})^T H_L\left(\boldsymbol{q}', \dot{\boldsymbol{q}}'\right) F_*(\boldsymbol{q})$$

where $F_*(\boldsymbol{q})^T$ is the transposed matrix, so that the condition $\det H_L \neq 0$ does not depend on the choice of standard coordinates.

For an invariant formulation, consider the 1-form θ_L, defined in standard coordinates associated with a coordinate chart $U \subset M$ by

$$\theta_L = \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}^i} dq^i = \frac{\partial L}{\partial \dot{\boldsymbol{q}}} d\boldsymbol{q}.$$

It follows from Corollary 1.2 that θ_L is a well-defined 1 -form on TM.

Lemma 1.2. A Lagrangian system (M, L) is non-degenerate if and only if the 2 -form $d\theta_L$ on TM is non-degenerate.

Proof. In standard coordinates,

$$d\theta_L = \sum_{i,j=1}^{n} \left(\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} d\dot{q}^j \wedge dq^i + \frac{\partial^2 L}{\partial \dot{q}^i \partial q^j} dq^j \wedge dq^i \right)$$

and it is easy to see, by considering the $2n$-form $d\theta_L^n = \underbrace{d\theta_L \wedge \cdots \wedge d\theta_L}_{n}$, that the 2-form $d\theta_L$ is non-degenerate if and only if the matrix H_L is nondegenerate.

Remark. Using the 1-form θ_L, the Noether integral I in Theorem 1.3 can be written as

$$I = i_{X'}(\theta_L) \tag{1.16}$$

where X' is a lift to TM of a vector field X on M given by (1.5). It also immediately follows from (1.6) that if X is an infinitesimal symmetry, then

$$\mathcal{L}_{X'}(\theta_L) = 0. \tag{1.17}$$

Definition. Let (U, φ) be a coordinate chart on M. Coordinates

$$(\boldsymbol{p}, \boldsymbol{q}) = \left(p_1, ..., p_n, q^1, ..., q^n\right)$$

on the chart $T^*U \simeq \mathbb{R}^n \times U$ on the cotangent bundle T^*M are called standard coordinates [14] if for $(p, q) \in T^*U$ and $f \in C^\infty(U)$

$$p_i(df) = \frac{\partial f}{\partial q^i}, \quad i = 1, ..., n$$

Equivalently, standard coordinates on T^*U are uniquely characterized by the condition that $\boldsymbol{p} = (p_1, ..., p_n)$ are coordinates in the fiber corresponding to the basis $dq^1, ..., dq^n$ for T_q^*M, dual to the basis $\frac{\partial}{\partial q^1}, ..., \frac{\partial}{\partial q^n}$ for T_qM.

Definition. The 1-form θ on T^*M, defined in standard coordinates by

$$\theta = \sum_{i=1}^{n} p_i dq^i = \boldsymbol{p} d\boldsymbol{q}$$

is called Liouville's canonical 1-form.

Corollary 1.2 shows that θ is a well-defined 1 -form on T^*M. Clearly, the 1 -form θ also admits an invariant definition

[014] Following tradition, the first n coordinates parametrize the fiber of T^*U and the last n coordinates parametrize the base.

$$\theta(u) = p\left(\pi_*(u)\right), \quad \text{where} \quad u \in T_{(p,q)}T^*M,$$

and $\pi : T^*M \to M$ is the canonical projection.

Definition. A fibre-wise mapping $\tau_L : TM \to T^*M$ is called a Legendre transform associated with the Lagrangian L if

$$\theta_L = \tau_L^*(\theta)$$

In standard coordinates the Legendre transform is given by

$$\tau_L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = (\boldsymbol{p}, \boldsymbol{q}), \quad \text{where} \quad \boldsymbol{p} = \frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}, \dot{\boldsymbol{q}}).$$

The mapping τ_L is a local diffeomorphism if and only if the Lagrangian L is non-degenerate.

Definition. Suppose that the Legendre transform $\tau_L : TM \to T^*M$ is a diffeomorphism. The Hamiltonian function $H : T^*M \to \mathbb{R}$, associated with the Lagrangian $L : TM \to \mathbb{R}$, is defined by

$$H \circ \tau_L = E_L = \dot{\boldsymbol{q}}\frac{\partial L}{\partial \dot{\boldsymbol{q}}} - L$$

In standard coordinates,

$$H(\boldsymbol{p}, \boldsymbol{q}) = \left(\boldsymbol{p}\dot{\boldsymbol{q}} - L(\boldsymbol{q}, \dot{\boldsymbol{q}})\right)\big|_{\boldsymbol{p}=\frac{\partial L}{\partial \dot{\boldsymbol{q}}}},$$

where $\dot{\boldsymbol{q}}$ is a function of $\boldsymbol{p}$ and $\boldsymbol{q}$ defined by the equation $\boldsymbol{p} = \frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}, \dot{\boldsymbol{q}})$ through the implicit function theorem. The cotangent bundle T^*M is called the phase space of the Lagrangian system (M, L). It turns out that on the phase space the equations of motion take a very simple and symmetric form.

Theorem 1.4. Suppose that the Legendre transform $\tau_L : TM \to T^*M$ is a diffeomorphism. Then the Euler-Lagrange equations in standard coordinates on TM,

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} - \frac{\partial L}{\partial q^i} = 0, \quad i = 1, ..., n$$

are equivalent to the following system of first order differential equations in standard coordinates on T^*M:

$$\dot{p}_i = -\frac{\partial H}{\partial q^i}, \quad \dot{q}^i = \frac{\partial H}{\partial p_i}, \quad i = 1, ..., n.$$

Proof. We have

$$\begin{aligned} dH &= \frac{\partial H}{\partial \boldsymbol{p}}d\boldsymbol{p} + \frac{\partial H}{\partial \boldsymbol{q}}d\boldsymbol{q} \\ &= \left(\boldsymbol{p}d\dot{\boldsymbol{q}} + \dot{\boldsymbol{q}}d\boldsymbol{p} - \frac{\partial L}{\partial \boldsymbol{q}}d\boldsymbol{q} - \frac{\partial L}{\partial \dot{\boldsymbol{q}}}d\dot{\boldsymbol{q}}\right)\Big|_{\boldsymbol{p}=\frac{\partial L}{\partial \dot{\boldsymbol{q}}}} \\ &= \left(\dot{\boldsymbol{q}}d\boldsymbol{p} - \frac{\partial L}{\partial \boldsymbol{q}}d\boldsymbol{q}\right)\Big|_{\boldsymbol{p}=\frac{\partial L}{\partial \dot{\boldsymbol{q}}}} \end{aligned}$$

Thus under the Legendre transform,

$$\dot{\boldsymbol{q}} = \frac{\partial H}{\partial \boldsymbol{p}} \quad \text{and} \quad \dot{\boldsymbol{p}} = \frac{d}{dt}\frac{\partial L}{\partial \dot{\boldsymbol{q}}} = \frac{\partial L}{\partial \boldsymbol{q}} = -\frac{\partial H}{\partial \boldsymbol{q}}.$$

Corresponding first order differential equations on T^*M are called Hamilton's equations (canonical equations).

Corollary 1.5. The Hamiltonian H is constant on the solutions of Hamilton's equations.

Proof. For $H(t) = H(\boldsymbol{p}(t), \boldsymbol{q}(t))$ we have

$$\frac{dH}{dt} = \frac{\partial H}{\partial \boldsymbol{q}}\dot{\boldsymbol{q}} + \frac{\partial H}{\partial \boldsymbol{p}}\dot{\boldsymbol{p}} = \frac{\partial H}{\partial \boldsymbol{q}}\frac{\partial H}{\partial \boldsymbol{p}} - \frac{\partial H}{\partial \boldsymbol{p}}\frac{\partial H}{\partial \boldsymbol{q}} = 0.$$

For the Lagrangian

$$L = \frac{m\dot{\boldsymbol{r}}^2}{2} - V(\boldsymbol{r}) = T - V, \quad \boldsymbol{r} \in \mathbb{R}^3,$$

of a particle of mass m in a potential field $V(\boldsymbol{r})$, considered in Example 1.4, we have

$$\boldsymbol{p} = \frac{\partial L}{\partial \dot{\boldsymbol{r}}} = m\dot{\boldsymbol{r}}.$$

Thus the Legendre transform $\tau_L : T\mathbb{R}^3 \to T^*\mathbb{R}^3$ is a global diffeomorphism, linear on the fibers, and

$$H(\boldsymbol{p}, \boldsymbol{r}) = (\boldsymbol{p}\dot{\boldsymbol{r}} - L)|_{\dot{\boldsymbol{r}} = \frac{\boldsymbol{p}}{m}} = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r}) = T + V$$

Hamilton's equations

$$\dot{\boldsymbol{r}} = \frac{\partial H}{\partial \boldsymbol{p}} = \frac{\boldsymbol{p}}{m}$$
$$\dot{\boldsymbol{p}} = -\frac{\partial H}{\partial r} = -\frac{\partial V}{\partial \boldsymbol{r}}$$

are equivalent to Newton's equations with the force $\boldsymbol{F} = -\frac{\partial V}{\partial \boldsymbol{r}}$.

For the Lagrangian system describing small oscillators, considered in Example 1.6, we have $\boldsymbol{p} = m\dot{\boldsymbol{q}}$, and using normal coordinates we get

$$H(\boldsymbol{p}, \boldsymbol{q}) = (\boldsymbol{p}\dot{\boldsymbol{q}} - L(\boldsymbol{q}, \dot{\boldsymbol{q}}))|_{\dot{\boldsymbol{q}} = \frac{\boldsymbol{p}}{m}} = \frac{\boldsymbol{p}^2}{2m} + V_0(\boldsymbol{q}) = \frac{1}{2m}\left(\boldsymbol{p}^2 + m^2 \sum_{i=1}^{n} \omega_i^2 \left(q^i\right)^2\right).$$

Similarly, for the system of N interacting particles, considered in Example 1.2, we have $\boldsymbol{p} = (\boldsymbol{p}_1, ..., \boldsymbol{p}_N)$, where

$$\boldsymbol{p}_a = \frac{\partial L}{\partial \dot{\boldsymbol{r}}_a} = m_a\dot{\boldsymbol{r}}_a, \quad a = 1, ..., N.$$

The Legendre transform $\tau_L : T\mathbb{R}^{3N} \to T^*\mathbb{R}^{3N}$ is a global diffeomorphism, linear on the fibers, and

$$H(\boldsymbol{p}, \boldsymbol{r}) = (\boldsymbol{p}\dot{\boldsymbol{r}} - L)|_{\dot{\boldsymbol{r}} = \frac{\boldsymbol{p}}{m}} = \sum_{a=1}^{N} \frac{\boldsymbol{p}_a^2}{2m_a} + V(\boldsymbol{r}) = T + V.$$

In particular, for a closed system with pair-wise interaction,

$$H(\boldsymbol{p}, \boldsymbol{r}) = \sum_{a=1}^{N} \frac{\boldsymbol{p}_a^2}{2m_a} + \sum_{1 \le a < b \le N} V_{ab}\left(\boldsymbol{r}_a - \boldsymbol{r}_b\right).$$

In general, consider the Lagrangian

$$L = \sum_{i,j=1}^{n} \frac{1}{2} a_{ij}(\boldsymbol{q}) \dot{q}^i \dot{q}^j - V(\boldsymbol{q}), \boldsymbol{q} \in \mathbb{R}^n,$$

where $A(\boldsymbol{q}) = \{a_{ij}(\boldsymbol{q})\}_{i,j=1}^n$ is a symmetric $n \times n$ matrix. We have

$$p_i = \frac{\partial L}{\partial \dot{q}^i} = \sum_{j=1}^{n} a_{ij}(\boldsymbol{q}) \dot{q}^j, \quad i = 1, ..., n,$$

and the Legendre transform is a global diffeomorphism, linear on the fibers, if and only if the matrix $A(\boldsymbol{q})$ is non-degenerate for all $\boldsymbol{q} \in \mathbb{R}^n$. In this case,

$$H(\boldsymbol{p}, \boldsymbol{q}) = (\boldsymbol{p}\dot{\boldsymbol{q}} - L(\boldsymbol{q}, \dot{\boldsymbol{q}}))|_{\boldsymbol{p}=\frac{\partial L}{\partial \dot{\boldsymbol{q}}}} = \sum_{i,j=1}^{n} \frac{1}{2} a^{ij}(\boldsymbol{q}) p_i p_j + V(\boldsymbol{q}),$$

where $\{a^{ij}(\boldsymbol{q})\}_{i,j=1}^n = A^{-1}(\boldsymbol{q})$ is the inverse matrix.

Problem 1.23 (Second tangent bundle). Let $\pi : TM \to M$ be the canonical projection and let $T_{\mathrm{V}}(TM)$ be the vertical tangent bundle of TM along the fibers of π - the kernel of the bundle mapping $\pi_* : T(TM) \to TM$. Prove that there is a natural bundle isomorphism $i : TM \simeq T_{\mathrm{V}}(TM)$.

Problem 1.24 (Invariant definition of the 1-form θ_L). Show that $\theta_L(v) = dL\left((i \circ \pi_*)\, v\right)$, where $v \in T(TM)$.

Problem 1.25. Give an invariant proof of (1.17).

Problem 1.26. Prove that the path $\gamma(t)$ in M is a trajectory for the Lagrangian system (M, L) if and only if

$$i_{\dot{\gamma}'(t)}\left(d\theta_L\right) + dE_L\left(\gamma'(t)\right) = 0,$$

where $\dot{\gamma}'(t)$ is the velocity vector of the path $\gamma'(t)$ in TM.

Problem 1.27. Show that for a charged particle in an electromagnetic field, considered in Example 1.5,

$$\boldsymbol{p} = m\dot{\boldsymbol{r}} + \frac{e}{c}\boldsymbol{A} \quad \text{and} \quad H(\boldsymbol{p}, \boldsymbol{r}) = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 + e\varphi(\boldsymbol{r}).$$

Problem 1.28. Suppose that for a Lagrangian system $(\mathbb{R}^n, L)$ the Legendre transform τ_L is a diffeomorphism and let H be the corresponding Hamiltonian. Prove that for fixed $\boldsymbol{q}$ and $\dot{\boldsymbol{q}}$ the function $\boldsymbol{p}\dot{\boldsymbol{q}} - H(\boldsymbol{p}, \boldsymbol{q})$ has a single critical point at $\boldsymbol{p} = \frac{\partial L}{\partial \dot{\boldsymbol{q}}}$.

Problem 1.29. Give an example of a non-degenerate Lagrangian system (M, L) such that the Legendre transform $\tau_L : TM \to T^*M$ is one-to-one but not onto.

2.12.2 2. Classical Hamiltonian Mechanics for QM 1

2.1. Hamilton's equations.

With every function $H : T^*M \to \mathbb{R}$ on the phase space T^*M there are associated Hamilton's equations - a first-order system of ordinary differential equations, which in the standard coordinates on T^*U has the form

$$\dot{\boldsymbol{p}} = -\frac{\partial H}{\partial \boldsymbol{q}}, \quad \dot{\boldsymbol{q}} = \frac{\partial H}{\partial \boldsymbol{p}}. \tag{2.1}$$

The corresponding vector field X_H on T^*U,

$$X_H = \sum_{i=1}^{n} \left(\frac{\partial H}{\partial p_i} \frac{\partial}{\partial q^i} - \frac{\partial H}{\partial q^i} \frac{\partial}{\partial p_i} \right) = \frac{\partial H}{\partial \boldsymbol{p}} \frac{\partial}{\partial \boldsymbol{q}} - \frac{\partial H}{\partial \boldsymbol{q}} \frac{\partial}{\partial \boldsymbol{p}}$$

gives rise to a well-defined vector field X_H on T^*M, called the Hamiltonian vector field. Suppose now that the vector field X_H on T^*M is complete, i.e., its integral curves exist for all times. The corresponding one-parameter group $\{g_t\}_{t\in\mathbb{R}}$ of diffeomorphisms of T^*M generated by X_H is called the Hamiltonian phase flow. It is defined by $g_t(p,q) = (p(t), q(t))$, where $p(t)$, $q(t)$ is a solution of Hamilton's equations satisfying $p(0) = p, q(0) = q$.

Liouville's canonical 1-form θ on T^*M defines a 2-form $\omega = d\theta$. In standard coordinates on T^*M it is given by

$$\omega = \sum_{i=1}^{n} dp_i \wedge dq^i = d\boldsymbol{p} \wedge d\boldsymbol{q}$$

and is a non-degenerate 2 -form. The form ω is called the canonical symplectic form on T^*M. The symplectic form ω defines an isomorphism J: $T^*\left(T^*M\right) \to T\left(T^*M\right)$ between tangent and cotangent bundles to T^*M. For every $(p,q) \in T^*M$ the linear mapping $J^{-1} : T_{(p,q)}T^*M \to T^*_{(p,q)}T^*M$ is given by

$$\omega\left(u_1, u_2\right) = J^{-1}\left(u_2\right)\left(u_1\right), \quad u_1, u_2 \in T_{(p,q)}T^*M$$

The mapping J induces the isomorphism between the infinite-dimensional vector spaces $\mathcal{A}^1\left(T^*M\right)$ and $\mathrm{Vect}\left(T^*M\right)$, which is linear over $C^\infty\left(T^*M\right)$. If ϑ is a 1 -form on T^*M, then the corresponding vector field $J(\vartheta)$ on T^*M satisfies

$$\omega(X, J(\vartheta)) = \vartheta(X), \quad X \in \mathrm{Vect}\left(T^*M\right)$$

and $J^{-1}(X) = -i_X\omega$. In particular, in standard coordinates,

$$J(d\boldsymbol{p}) = \frac{\partial}{\partial \boldsymbol{q}} \quad \text{and} \quad J(d\boldsymbol{q}) = -\frac{\partial}{\partial \boldsymbol{p}}$$

so that $X_H = J(dH)$.

Theorem 2.1. The Hamiltonian phase flow on T^*M preserves the canonical symplectic form.

Proof. We need to prove that $\left(g_t\right)^* \omega = \omega$. Since g_t is a one-parameter group of diffeomorphisms, it is sufficient to show that

$$\frac{d}{dt}\left(g_t\right)^* \omega \Big|_{t=0} = \mathcal{L}_{X_H}\omega = 0$$

where $\mathcal{L}_{X_H}$ is the Lie derivative along the vector field X_H. Since for every vector field X,

$$\mathcal{L}_X(df) = d(X(f)),$$

we compute

$$\mathcal{L}_{X_H}\left(dp_i\right) = -d\left(\frac{\partial H}{\partial q^i}\right) \quad \text{and} \quad \mathcal{L}_{X_H}\left(dq^i\right) = d\left(\frac{\partial H}{\partial p_i}\right)$$

so that

$$\begin{aligned}
\mathcal{L}_{X_H}\omega &= \sum_{i=1}^{n} \left(\mathcal{L}_{X_H}\left(dp_i\right) \wedge dq^i + dp_i \wedge \mathcal{L}_{X_H}\left(dq^i\right) \right) \\
&= \sum_{i=1}^{n} \left(-d\left(\frac{\partial H}{\partial q^i}\right) \wedge dq^i + dp_i \wedge d\left(\frac{\partial H}{\partial p_i}\right) \right) = -d(dH) = 0.
\end{aligned}$$

Corollary 2.2. $\mathcal{L}_{X_H}(\theta) = d\left(-H + \theta\left(X_H\right)\right)$, where θ is Liouville's canonical 1-form.

The canonical symplectic form ω on T^*M defines the volume form $\frac{\omega^n}{n!} = \frac{1}{n!}\underbrace{\omega \wedge \cdots \wedge \omega}_{n}$ on T^*M, called Liouville's volume form.

Corollary 2.3 (Liouville's theorem). The Hamiltonian phase flow on T^*M preserves Liouville's volume form.

The restriction of the symplectic form ω on T^*M to the configuration space M is 0 . Generalizing this property, we get the following notion.

Definition. A submanifold $\mathscr{L}$ of the phase space T^*M is called a *La* grangian submanifold if $\dim \mathscr{L} = \dim M$ and $\omega|_{\mathscr{L}} = 0$.

It follows from Theorem 2.1 that the image of a Lagrangian submanifold under the Hamiltonian phase flow is a Lagrangian submanifold.

Problem 2.1. Verify that X_H is a well-defined vector field on T^*M.

Problem 2.2. Show that if all level sets of the Hamiltonian H are compact submanifolds of T^*M, then the Hamiltonian vector field X_H is complete.

Problem 2.3. Let $\pi : T^*M \to M$ be the canonical projection, and let $\mathscr{L}$ be a Lagrangian submanifold. Show that if the mapping $\pi|_{\mathscr{L}} : \mathscr{L} \to M$ is a diffeomorphism, then $\mathscr{L}$ is a graph of a smooth function on M. Give examples when for some $t > 0$ the corresponding projection of $g_t(\mathscr{L})$ onto M is no longer a diffeomorphism.

2.2. The action functional in the phase space.

With every function H on the phase space T^*M there is an associated 1-form

$$\theta - Hdt = \boldsymbol{p}d\boldsymbol{q} - Hdt$$

on the extended phase space $T^*M \times \mathbb{R}$, called the Poincar-Cartan form. Let $\gamma : [t_0, t_1] \to T^*M$ be a smooth parametrized path in T^*M such that $\pi\left(\gamma\left(t_0\right)\right) = q_0$ and $\pi\left(\gamma\left(t_1\right)\right) = q_1$, where $\pi : T^*M \to M$ is the canonical projection. By definition, the lift of a path γ to the extended phase space $T^*M \times \mathbb{R}$ is a path $\sigma : [t_0, t_1] \to T^*M \times \mathbb{R}$ given by $\sigma(t) = (\gamma(t), t)$, and a path σ in $T^*M \times \mathbb{R}$ is called an admissible path if it is a lift of a path γ in T^*M. The space of admissible paths in $T^*M \times \mathbb{R}$ is denoted by $\tilde{P}\left(T^*M\right)_{q_0,t_0}^{q_1,t_1}$. A variation of an admissible path σ is a smooth family of admissible paths σ_ε, where $\varepsilon \in [-\varepsilon_0, \varepsilon_0]$ and $\sigma_0 = \sigma$, and the corresponding infinitesimal variation is

$$\delta\sigma = \left.\frac{\partial \sigma_\varepsilon}{\partial \varepsilon}\right|_{\varepsilon=0} \in T_\sigma \tilde{P}\left(T^*M\right)_{q_0,t_0}^{q_1,t_1}$$

(cf. Section 1.2). The principle of the least action in the phase space is the following statement.

Theorem 2.4 (Poincar). The admissible path σ in $T^*M \times \mathbb{R}$ is an extremal for the action functional

$$S(\sigma) = \int_\sigma (\boldsymbol{p}d\boldsymbol{q} - Hdt) = \int_{t_0}^{t_1} (\boldsymbol{p}\dot{\boldsymbol{q}} - H)dt$$

if and only if it is a lift of a path $\gamma(t) = (\boldsymbol{p}(t), \boldsymbol{q}(t))$ in T^*M, where $\boldsymbol{p}(t)$ and $\boldsymbol{q}(t)$ satisfy canonical Hamilton's equations

$$\dot{\boldsymbol{p}} = -\frac{\partial H}{\partial \boldsymbol{q}}, \quad \dot{\boldsymbol{q}} = \frac{\partial H}{\partial \boldsymbol{p}}$$

Proof. As in the proof of Theorem 1.1, for an admissible family $\sigma_\varepsilon(t) = (\boldsymbol{p}(t,\varepsilon), \boldsymbol{q}(t,\varepsilon), t)$ we compute using integration by parts,

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} S(\sigma_\varepsilon) = \sum_{i=1}^{n} \int_{t_0}^{t_1} \left(\dot{q}^i \delta p_i - \dot{p}_i \delta q^i - \frac{\partial H}{\partial q^i} \delta q^i - \frac{\partial H}{\partial p_i} \delta p_i \right) dt + \sum_{i=1}^{n} p_i \delta q^i \Big|_{t_0}^{t_1}$$

Since $\delta \boldsymbol{q}(t_0) = \delta \boldsymbol{q}(t_1) = 0$, the path σ is critical if and only if $\boldsymbol{p}(t)$ and $\boldsymbol{q}(t)$ satisfy canonical Hamilton's equations (2.1).

Remark. For a Lagrangian system (M, L), every path $\gamma(t) = (\boldsymbol{q}(t))$ in the configuration space M connecting points q_0 and q_1 defines an admissible path $\hat{\gamma}(t) = (\boldsymbol{p}(t), \boldsymbol{q}(t), t)$ in the phase space T^*M by setting $\boldsymbol{p} = \frac{\partial L}{\partial \dot{\boldsymbol{q}}}$. If the Legendre transform $\tau_L : TM \to T^*M$ is a diffeomorphism, then

$$S(\hat{\gamma}) = \int_{t_0}^{t_1} (\boldsymbol{p}\dot{\boldsymbol{q}} - H) dt = \int_{t_0}^{t_1} L(\gamma'(t), t)\, dt$$

Thus the principle of the least action in a configuration space - Hamilton's principle - follows from the principle of the least action in a phase space. In fact, in this case the two principles are equivalent (see Problem 1.28).

From Corollary 1.5 we immediately get the following result.

Corollary 2.5. Solutions of canonical Hamilton's equations lying on the hypersurface $H(\boldsymbol{p}, \boldsymbol{q}) = E$ are extremals of the functional $\int_\sigma \boldsymbol{p} d\boldsymbol{q}$ in the class of admissible paths σ lying on this hypersurface.

Corollary 2.6 (Maupertuis' principle). The trajectory $\gamma = (\boldsymbol{q}(\tau))$ of a closed Lagrangian system (M, L) connecting points q_0 and q_1 and having energy E is the extremal of the functional

$$\int_\gamma \boldsymbol{p} d\boldsymbol{q} = \int_\gamma \frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}(\tau), \dot{\boldsymbol{q}}(\tau)) \dot{\boldsymbol{q}}(\tau) d\tau$$

on the space of all paths in the configuration space M connecting points q_0 and q_1 and parametrized such that $H\left(\frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\tau), \boldsymbol{q}(\tau)\right) = E$.

The functional

$$S_0(\gamma) = \int_\gamma \boldsymbol{p} d\boldsymbol{q}$$

is called the abbreviated action [15].

Proof. Every path $\gamma = \boldsymbol{q}(\tau)$, parametrized such that $H\left(\frac{\partial L}{\partial \dot{\boldsymbol{q}}}, \boldsymbol{q}\right) = E$, lifts to an admissible path $\sigma = \left(\frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\tau), \boldsymbol{q}(\tau), \tau\right), a \le \tau \le b$, lying on the hypersurface $H(\boldsymbol{p}, \boldsymbol{q}) = E$.

Problem 2.4 (Jacobi). On a Riemannian manifold (M, ds^2) consider a Lagrangian system with $L(q, v) = \frac{1}{2}\|v\|^2 - V(q)$. Let $E > V(q)$ for all $q \in M$. Show that the trajectories of a closed Lagrangian system (M, L) with total energy E are geodesics for the Riemannian metric $d\hat{s}^2 = (E - V(q)) ds^2$ on M.

2.3. The action as a function of coordinates.

Consider a non-degenerate Lagrangian system (M, L) and denote by $\gamma(t; q_0, v_0)$ the solution of Euler-Lagrange equations

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\boldsymbol{q}}} - \frac{\partial L}{\partial \boldsymbol{q}} = 0$$

with the initial conditions $\gamma(t_0) = q_0 \in M$ and $\dot{\gamma}(t_0) = v_0 \in T_{q_0}M$. Suppose that there exist a neighborhood $V_0 \subset T_{v_0}M$ of v_0 and $t_1 > t_0$ such that for all $v \in V_0$ the extremals $\gamma(t; q_0, v)$, which start at time t_0 at q_0, do not intersect in the extended configuration space $M \times \mathbb{R}$ for times $t_0 < t < t_1$. Such extremals are said to form a central field which includes the extremal $\gamma_0(t) = \gamma(t; q_0, v_0)$. The existence of the central field of extremals is equivalent to the condition that for every $t_0 < t < t_1$ there is a neighborhood $U_t \subset M$ of $\gamma_0(t) \in M$ such that the mapping

$$V_0 \ni v \mapsto q(t) = \gamma(t; q_0, v) \in U_t \tag{2.2}$$

is a diffeomorphism. Basic theorems in the theory of ordinary differential equations guarantee that for t_1 sufficiently close to t_0 every extremal $\gamma(t)$ for $t_0 < t < t_1$ can be included into the central field. In standard coordinates the mapping (2.2) is given by $\dot{\boldsymbol{q}} \mapsto \boldsymbol{q}(t) = \gamma(t; \boldsymbol{q}_0, \dot{\boldsymbol{q}})$.

For the central field of extremals $\gamma(t; \boldsymbol{q}_0, \dot{\boldsymbol{q}}), t_0 < t < t_1$, we define the action as a function of coordinates and time (or, classical action) by

$$S(\boldsymbol{q}, t; \boldsymbol{q}_0, t_0) = \int_{t_0}^{t} L(\gamma'(\tau))\, d\tau$$

where $\gamma(\tau)$ is the extremal from the central field that connects $\boldsymbol{q}_0$ and $\boldsymbol{q}$. For given $\boldsymbol{q}_0$ and t_0, the classical action is defined for $t \in (t_0, t_1)$ and $\boldsymbol{q} \in \bigcup_{t_0<t<t_1} U_t$. For a fixed energy E,

$$S(\boldsymbol{q}, t; \boldsymbol{q}_0, t_0) = S_0(\boldsymbol{q}, t; \boldsymbol{q}_0, t_0) - E(t - t_0), \tag{2.3}$$

where S_0 is the abbreviated action from the previous section. Theorem 2.7. The differential of the classical action $S(\boldsymbol{q}, t)$ with fixed initial point is given by

$$dS = \boldsymbol{p}d\boldsymbol{q} - Hdt$$

where $\boldsymbol{p} = \frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q}, \dot{\boldsymbol{q}})$ and $H = \boldsymbol{p}\dot{\boldsymbol{q}} - L(\boldsymbol{q}, \dot{\boldsymbol{q}})$ are determined by the velocity $\dot{\boldsymbol{q}}$ of the extremal $\gamma(\tau)$ at time t.

Proof. Let $\boldsymbol{q}_\varepsilon$ be a path in M passing through $\boldsymbol{q}$ at $\varepsilon = 0$ with the tangent vector $v \in T_{\boldsymbol{q}}M \simeq \mathbb{R}^n$, and for ε small enough let $\gamma_\varepsilon(\tau)$ be the family of extremals from the central field satisfying $\gamma_\varepsilon(t_0) = \boldsymbol{q}_0$ and $\gamma_\varepsilon(t) = \boldsymbol{q}_\varepsilon$. For the infinitesimal variation $\delta\gamma$ we have $\delta\gamma(t_0) = 0$ and $\delta\gamma(t) = \boldsymbol{v}$, and for fixed t we get from the formula for variation with the free ends (1.2) that

$$dS(\boldsymbol{v}) = \frac{\partial L}{\partial \dot{\boldsymbol{q}}}\boldsymbol{v}.$$

This shows that $\frac{\partial S}{\partial \boldsymbol{q}} = \boldsymbol{p}$. Setting $\boldsymbol{q}(t) = \gamma(t)$, we obtain

$$\frac{d}{dt}S(\boldsymbol{q}(t), t) = \frac{\partial S}{\partial \boldsymbol{q}}\dot{\boldsymbol{q}} + \frac{\partial S}{\partial t} = L,$$

so that $\frac{\partial S}{\partial t} = L - \boldsymbol{p}\dot{\boldsymbol{q}} = -H$.

Corollary 2.8. The classical action satisfies the following nonlinear partial differential equation

$$\frac{\partial S}{\partial t} + H\left(\frac{\partial S}{\partial \boldsymbol{q}}, \boldsymbol{q}\right) = 0 \tag{2.4}$$

[015] The accurate formulation of Maupertuis' principle is due to Euler and Lagrange.

This equation is called the Hamilton-Jacobi equation. Hamilton's equations (2.1) can be used for solving the Cauchy problem

$$S(\boldsymbol{q},t)|_{t=0} = s(\boldsymbol{q}), \quad s \in C^\infty(M), \tag{2.5}$$

for Hamilton-Jacobi equation (2.4) by the method of characteristics. Namely, assume the existence of the Hamiltonian phase flow g_t on T^*M and consider the Lagrangian submanifold

$$\mathscr{L} = \left\{ (\boldsymbol{p},\boldsymbol{q}) \in T^*M : \boldsymbol{p} = \frac{\partial s(\boldsymbol{q})}{\partial \boldsymbol{q}} \right\},$$

a graph of the 1 -form ds on M - a section of the cotangent bundle π: $T^*M \to M$. The mapping $\pi|_{\mathscr{L}}$ is one-to-one and for sufficiently small t the restriction of the projection π to the Lagrangian submanifold $\mathscr{L}_t = g_t(\mathscr{L})$ remains to be one-to-one. In other words, there is $t_1 > 0$ such that for all $0 \le t < t_1$ the mapping $\pi_t = \pi \circ g_t \circ (\pi|_{\mathscr{L}})^{-1} : M \to M$ is a diffeomorphism, and the extremals $\gamma(\tau, \boldsymbol{q}_0, \dot{\boldsymbol{q}}_0)$ in the extended configuration space $M \times \mathbb{R}$, where $\dot{\boldsymbol{q}}_0 = \frac{\partial H}{\partial \boldsymbol{p}}(\boldsymbol{p}_0, \boldsymbol{q}_0)$ and $(\boldsymbol{p}_0, \boldsymbol{q}_0) \in \mathscr{L}$, do not intersect. Such extremals are called the characteristics of the Hamilton-Jacobi equation.

Proposition 2.1. For $0 \le t < t_1$ the solution $S(\boldsymbol{q},t)$ to the Cauchy problem (2.4)-(2.5) is given by

$$S(\boldsymbol{q},t) = s(\boldsymbol{q}_0) + \int_0^t L(\gamma'(\tau))\, d\tau$$

Here $\gamma(\tau)$ is the characteristic with $\gamma(t) = \boldsymbol{q}$ and with the starting point $\boldsymbol{q}_0 = \gamma(0)$ which is uniquely determined by $\boldsymbol{q}$.

Proof. As in the proof of Theorem 2.7 we use formula (1.2), where now $\boldsymbol{q}_0$ depends on $\boldsymbol{q}$, and obtain

$$\frac{\partial S}{\partial \boldsymbol{q}}(\boldsymbol{q}) = \frac{\partial s}{\partial \boldsymbol{q}_0}(\boldsymbol{q}_0)\frac{\partial \boldsymbol{q}_0}{\partial \boldsymbol{q}} + \frac{\partial L}{\partial \dot{\boldsymbol{q}}}(\boldsymbol{q},\dot{\boldsymbol{q}}) - \frac{\partial L}{\partial \dot{\boldsymbol{q}}_0}(\boldsymbol{q}_0,\dot{\boldsymbol{q}}_0)\frac{\partial \boldsymbol{q}_0}{\partial \boldsymbol{q}} = \boldsymbol{p}$$

since $\frac{\partial s}{\partial \boldsymbol{q}_0}(\boldsymbol{q}_0) = \boldsymbol{p}_0 = \frac{\partial L}{\partial \dot{\boldsymbol{q}}_0}(\boldsymbol{q}_0,\dot{\boldsymbol{q}}_0)$. Setting $\boldsymbol{q}(t) = \gamma(t)$ we get

$$\frac{d}{dt}S(\boldsymbol{q}(t),t) = \frac{\partial S}{\partial \boldsymbol{q}}\dot{\boldsymbol{q}} + \frac{\partial S}{\partial t} = L(\boldsymbol{q},\dot{\boldsymbol{q}})$$

so that

$$\frac{\partial S}{\partial t} = -H(\boldsymbol{p},\boldsymbol{q})$$

and S satisfies the Hamilton-Jacobi equation.

We can also consider the action $S(\boldsymbol{q},t;\boldsymbol{q}_0,t_0)$ as a function of both variables $\boldsymbol{q}$ and $\boldsymbol{q}_0$. The analog of Theorem 2.7 is the following statement.

Proposition 2.2. The differential of the classical action as a function of initial and final points is given by

$$dS = \boldsymbol{p}d\boldsymbol{q} - \boldsymbol{p}_0 d\boldsymbol{q}_0 - H(\boldsymbol{p},\boldsymbol{q})dt + H(\boldsymbol{p}_0,\boldsymbol{q}_0)\,dt_0$$

Problem 2.5. Prove that the solution to the Cauchy problem for the HamiltonJacobi equation is unique.

2.12.3 2. Classical Hamiltonian Mechanics for QM 2

2.4. Classical observables and Poisson bracket.

Smooth real-valued functions on the phase space T^*M are called classical observables. The vector space $C^\infty(T^*M)$ is an $\mathbb{R}$-algebra - an associative algebra over $\mathbb{R}$ with a unit given by the constant function 1, and with a multiplication given by the point-wise product of functions. The commutative algebra $C^\infty(T^*M)$ is called the algebra of classical observables. Assuming that the Hamiltonian phase flow g_t exists for all times, the time evolution of every observable $f \in C^\infty(T^*M)$ is given by

$$f_t(p,q) = f(g_t(p,q)) = f(p(t),q(t)), \quad (p,q) \in TM$$

Equivalently, the time evolution is described by the differential equation

$$\begin{aligned}\frac{df_t}{dt} &= \left.\frac{df_{s+t}}{ds}\right|_{s=0} = \left.\frac{d(f_t \circ g_s)}{ds}\right|_{s=0} = X_H(f_t) \\ &= \sum_{i=1}^{n}\left(\frac{\partial H}{\partial p_i}\frac{\partial f_t}{\partial q^i} - \frac{\partial H}{\partial q^i}\frac{\partial f_t}{\partial p_i}\right) = \frac{\partial H}{\partial \boldsymbol{p}}\frac{\partial f_t}{\partial \boldsymbol{q}} - \frac{\partial H}{\partial \boldsymbol{q}}\frac{\partial f_t}{\partial \boldsymbol{p}},\end{aligned}$$

called Hamilton's equation for classical observables. Setting

$$\{f,g\} = X_f(g) = \frac{\partial f}{\partial \boldsymbol{p}}\frac{\partial g}{\partial \boldsymbol{q}} - \frac{\partial f}{\partial \boldsymbol{q}}\frac{\partial g}{\partial \boldsymbol{p}}, \quad f,g \in C^\infty(T^*M) \tag{2.6}$$

we can rewrite Hamilton's equation in the concise form

$$\frac{df}{dt} = \{H,f\} \tag{2.7}$$

where it is understood that (2.7) is a differential equation for a family of functions f_t on T^*M with the initial condition $f_t(p,q)|_{t=0} = f(p,q)$. The properties of the bilinear mapping

$$\{,\} : C^\infty(T^*M) \times C^\infty(T^*M) \to C^\infty(T^*M)$$

are summarized below.

Theorem 2.9. The mapping $\{,\}$ *satisfies the following properties.*

(i) (Relation with the symplectic form)

$$\{f,g\} = \omega(J(df), J(dg)) = \omega(X_f, X_g)$$

(ii) (Skew-symmetry)

$$\{f,g\} = -\{g,f\}$$

(iii) (Leibniz rule)

$$\{fg,h\} = f\{g,h\} + g\{f,h\}.$$

(iv) (Jacobi identity)

$$\{f,\{g,h\}\} + \{g,\{h,f\}\} + \{h,\{f,g\}\} = 0$$

for all $f,g,h \in C^\infty(T^*M)$.

Proof. Property (i) immediately follows from the definitions of ω and J in Section 2.1. Properties (ii)-(iii) are obvious. The Jacobi identity could be verified by a direct computation using (2.6), or by the following elegant argument. Observe that $\{f,g\}$ is a bilinear form in the

first partial derivatives of f and g, and every term in the left-hand side of the Jacobi identity is a linear homogenous function of second partial derivatives of f, g, and h. Now the only terms in the Jacobi identity which could actually contain second partial derivatives of a function h are the following:

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} = (X_f X_g - X_g X_f)(h)$$

However, this expression does not contain second partial derivatives of h since it is a commutator of two differential operators of the first order which is again a differential operator of the first order!

The observable $\{f, g\}$ is called the canonical Poisson bracket of the observables f and g. The Poisson bracket map $\{\} :, C^\infty(T^*M) \times C^\infty(T^*M) \to C^\infty(T^*M)$ turns the algebra of classical observables $C^\infty(T^*M)$ into a Lie algebra with a Lie bracket given by the Poisson bracket. It has an important property that the Lie bracket is a bi-derivation with respect to the multiplication in $C^\infty(T^*M)$. The algebra of classical observables $C^\infty(T^*M)$ is an example of the Poisson algebra - a commutative algebra over $\mathbb{R}$ carrying a structure of a Lie algebra with the property that the Lie bracket is a derivation with respect to the algebra product.

In Lagrangian mechanics, a function I on TM is an integral of motion for the Lagrangian system (M, L) if it is constant along the trajectories. In Hamiltonian mechanics, an observable I - a function on the phase space T^*M - is called an integral of motion (first integral) for Hamilton's equations (2.1) if it is constant along the Hamiltonian phase flow. According to (2.7), this is equivalent to the condition

$$\{H, I\} = 0$$

It is said that the observables H and I are in involution (Poisson commute).

2.5. Canonical transformations and generating functions.

Definition. A diffeomorphism g of the phase space T^*M is called a canonical transformation, if it preserves the canonical symplectic form ω on T^*M, i.e., $g^*(\omega) = \omega$. By Theorem 2.1, the Hamiltonian phase flow g_t is a oneparameter group of canonical transformations.

Proposition 2.3. Canonical transformations preserve Hamilton's equations.

Proof. From $g^*(\omega) = \omega$ it follows that the mapping $J : T^*(T^*M) \to T(T^*M)$ satisfies

$$g_* \circ J \circ g^* = J. \tag{2.8}$$

Indeed, for all $X, Y \in \mathrm{Vect}(M)$ we have [16]

$$\omega(X, Y) = g^*(\omega)(X, Y) = \omega(g_*(X), g_*(Y)) \circ g$$

so that for every 1 -form ϑ on M,

$$\omega(X, J(g^*(\vartheta))) = g^*(\vartheta)(X) = \vartheta(g_*(X)) \circ g = \omega(g_*(X), J(\vartheta)) \circ g$$

which gives $g_*(J(g^*(\vartheta))) = J(\vartheta)$. Using (2.8), we get

$$g_*(X_H) = g_*(J(dH)) = J\left((g^*)^{-1}(dH)\right) = X_K,$$

where $K = H \circ g^{-1}$. Thus the canonical transformation g maps trajectories of the Hamiltonian vector field X_H into the trajectories of the Hamiltonian vector field X_K.

Remark. In classical terms, Proposition 2.3 means that canonical Hamilton's equations

$$\dot{\boldsymbol{p}} = -\frac{\partial H}{\partial \boldsymbol{q}}(\boldsymbol{p}, \boldsymbol{q}), \quad \dot{\boldsymbol{q}} = \frac{\partial H}{\partial \boldsymbol{p}}(\boldsymbol{p}, \boldsymbol{q})$$

in new coordinates $(\boldsymbol{P}, \boldsymbol{Q}) = g(\boldsymbol{p}, \boldsymbol{q})$ continue to have the canonical form

$$\dot{\boldsymbol{P}} = -\frac{\partial K}{\partial \boldsymbol{Q}}(\boldsymbol{P}, \boldsymbol{Q}), \quad \dot{\boldsymbol{Q}} = \frac{\partial K}{\partial \boldsymbol{P}}(\boldsymbol{P}, \boldsymbol{Q})$$

with the old Hamiltonian function $K(\boldsymbol{P}, \boldsymbol{Q}) = H(\boldsymbol{p}, \boldsymbol{q})$.

Consider now the classical case $M = \mathbb{R}^n$. For a canonical transformation $(\boldsymbol{P}, \boldsymbol{Q}) = g(\boldsymbol{p}, \boldsymbol{q})$ set $\boldsymbol{P} = \boldsymbol{P}(\boldsymbol{p}, \boldsymbol{q})$ and $\boldsymbol{Q} = \boldsymbol{Q}(\boldsymbol{p}, \boldsymbol{q})$. Since $d\boldsymbol{P} \wedge d\boldsymbol{Q} = d\boldsymbol{p} \wedge d\boldsymbol{q}$ on $T^*M \simeq \mathbb{R}^{2n}$, the 1-form $\boldsymbol{p}d\boldsymbol{q} - \boldsymbol{P}d\boldsymbol{Q}$ - the difference between the canonical Liouville 1-form and its pullback by the mapping g-is closed. From the Poincar lemma it follows that there exists a function $F(\boldsymbol{p}, \boldsymbol{q})$ on $\mathbb{R}^{2n}$ such that

$$\boldsymbol{p}d\boldsymbol{q} - \boldsymbol{P}d\boldsymbol{Q} = dF(\boldsymbol{p}, \boldsymbol{q}) \tag{2.9}$$

Now assume that at some point $(\boldsymbol{p}_0, \boldsymbol{q}_0)$ the $n \times n$ matrix $\frac{\partial \boldsymbol{P}}{\partial \boldsymbol{p}} = \left\{ \frac{\partial P_i}{\partial p_j} \right\}_{i,j=1}^{n}$ is non-degenerate. By the inverse function theorem, there exists a neighborhood U of $(\boldsymbol{p}_0, \boldsymbol{q}_0)$ in $\mathbb{R}^{2n}$ for which the functions $\boldsymbol{P}, \boldsymbol{q}$ are coordinate functions. The function

$$S(\boldsymbol{P}, \boldsymbol{q}) = F(\boldsymbol{p}, \boldsymbol{q}) + \boldsymbol{P}\boldsymbol{Q}$$

is called a generating function of the canonical transformation g in U. It follows from (2.9) that in new coordinates $\boldsymbol{P}, \boldsymbol{q}$ on U,

$$\boldsymbol{p} = \frac{\partial S}{\partial \boldsymbol{q}}(\boldsymbol{P}, \boldsymbol{q}) \quad \text{and} \quad \boldsymbol{Q} = \frac{\partial S}{\partial \boldsymbol{P}}(\boldsymbol{P}, \boldsymbol{q})$$

The converse statement below easily follows from the implicit function theorem.

Proposition 2.4. Let $S(\boldsymbol{P}, \boldsymbol{q})$ be a function in some neighborhood U of a point $(\boldsymbol{P}_0, \boldsymbol{q}_0) \in \mathbb{R}^{2n}$ such that the $n \times n$ matrix

$$\frac{\partial^2 S}{\partial \boldsymbol{P} \partial \boldsymbol{q}}(\boldsymbol{P}_0, \boldsymbol{q}_0) = \left\{ \frac{\partial^2 S}{\partial P_i \partial q^j}(\boldsymbol{P}_0, \boldsymbol{q}_0) \right\}_{i,j=1}^{n}$$

is non-degenerate. Then S is a generating function of a local (i.e., defined in some neighborhood of $(\boldsymbol{P}_0, \boldsymbol{q}_0)$ in $\mathbb{R}^{2n}$) canonical transformation.

Suppose there is a canonical transformation $(\boldsymbol{P}, \boldsymbol{Q}) = g(\boldsymbol{p}, \boldsymbol{q})$ such that $H(\boldsymbol{p}, \boldsymbol{q}) = K(\boldsymbol{P})$ for some function K. Then in the new coordinates Hamilton's equations take the form

$$\dot{\boldsymbol{P}} = 0, \quad \dot{\boldsymbol{Q}} = \frac{\partial K}{\partial \boldsymbol{P}} \tag{2.10}$$

and are trivially integrated:

$$\boldsymbol{P}(t) = \boldsymbol{P}(0), \quad \boldsymbol{Q}(t) = \boldsymbol{Q}(0) + t\frac{\partial K}{\partial \boldsymbol{P}}(\boldsymbol{P}(0))$$

Assuming that the matrix $\frac{\partial \boldsymbol{P}}{\partial \boldsymbol{p}}$ is non-degenerate, the generating function $S(\boldsymbol{P}, \boldsymbol{q})$ satisfies the differential equation

$$H\left(\frac{\partial S}{\partial \boldsymbol{q}}(\boldsymbol{P}, \boldsymbol{q}), \boldsymbol{q}\right) = K(\boldsymbol{P}) \tag{2.11}$$

[016] Since g is a diffeomorphism, g_*X is a well-defined vector field on M.

where after the differentiation one should substitute $\boldsymbol{q} = \boldsymbol{q}(\boldsymbol{P}, \boldsymbol{Q})$, defined by the canonical transformation g^{-1}. The differential equation (2.11) for fixed $\boldsymbol{P}$, as it follows from (2.3), coincides with the Hamilton-Jacobi equation for the abbreviated action $S_0 = S - Et$ where $E = K(\boldsymbol{P})$,

$$H\left(\frac{\partial S_0}{\partial \boldsymbol{q}}(\boldsymbol{P}, \boldsymbol{q}), \boldsymbol{q}\right) = E$$

Theorem 2.10 (Jacobi). Suppose that there is a function $S(\boldsymbol{P}, \boldsymbol{q})$ which depends on n parameters $\boldsymbol{P} = (P_1, ..., P_n)$, satisfies the Hamilton-Jacobi equation (2.11) for some function $K(\boldsymbol{P})$, and has the property that the $n \times n$ matrix $\frac{\partial^2 S}{\partial \boldsymbol{P} \partial \boldsymbol{q}}$ is non-degenerate. Then Hamilton's equations

$$\dot{\boldsymbol{p}} = -\frac{\partial H}{\partial \boldsymbol{q}}, \quad \dot{\boldsymbol{q}} = \frac{\partial H}{\partial \boldsymbol{p}}$$

can be solved explicitly, and the functions $\boldsymbol{P}(\boldsymbol{p}, \boldsymbol{q}) = (P_1(\boldsymbol{p}, \boldsymbol{q}), ..., P_n(\boldsymbol{p}, \boldsymbol{q}))$, defined by the equations $\boldsymbol{p} = \frac{\partial S}{\partial \boldsymbol{q}}(\boldsymbol{P}, \boldsymbol{q})$, are integrals of motion in involution.

Proof. Set $\boldsymbol{p} = \frac{\partial S}{\partial \boldsymbol{q}}(\boldsymbol{P}, \boldsymbol{q})$ and $\boldsymbol{Q} = \frac{\partial S}{\partial \boldsymbol{P}}(\boldsymbol{P}, \boldsymbol{q})$. By the inverse function theorem, $g(\boldsymbol{p}, \boldsymbol{q}) = (\boldsymbol{P}, \boldsymbol{Q})$ is a local canonical transformation with the generating function S. It follows from (2.11) that $H(\boldsymbol{p}(\boldsymbol{P}, \boldsymbol{Q}), \boldsymbol{q}(\boldsymbol{P}, \boldsymbol{Q})) = K(\boldsymbol{P})$, so that Hamilton's equations take the form (2.10). Since $\omega = d\boldsymbol{P} \wedge d\boldsymbol{Q}$, integrals of motion $P_1(\boldsymbol{p}, \boldsymbol{q}), ..., P_n(\boldsymbol{p}, \boldsymbol{q})$ are in involution.

The solution of the Hamilton-Jacobi equation satisfying conditions in Theorem 2.10 is called the complete integral. At first glance it seems that solving the Hamilton-Jacobi equation, which is a nonlinear partial differential equation, is a more difficult problem then solving Hamilton's equations, which is a system of ordinary differential equations. It is quite remarkable that for many problems of classical mechanics one can find the complete integral of the Hamilton-Jacobi equation by the method of separation of variables. By Theorem 2.10, this solves the corresponding Hamilton's equations.

Problem 2.6. Find the generating function for the identity transformation $\boldsymbol{P} = p, Q = q$.

Problem 2.7. Prove Proposition 2.4.

Problem 2.8. Suppose that the canonical transformation $g(\boldsymbol{p}, \boldsymbol{q}) = (\boldsymbol{P}, \boldsymbol{Q})$ is such that locally $(\boldsymbol{Q}, \boldsymbol{q})$ can be considered as new coordinates (canonical transformations with this property are called free). Prove that $S_1(\boldsymbol{Q}, \boldsymbol{q}) = F(\boldsymbol{p}, \boldsymbol{q})$, also called a generating function, satisfies

$$\boldsymbol{p} = \frac{\partial S_1}{\partial \boldsymbol{q}} \quad \text{and} \quad \boldsymbol{P} = -\frac{\partial S_1}{\partial \boldsymbol{Q}}$$

Problem 2.9. Find the complete integral for the case of a particle in $\mathbb{R}^3$ moving in a central field.

2.6. Symplectic manifolds. The notion of a symplectic manifold is a generalization of the example of a cotangent bundle T^*M.

Definition. A non-degenerate, closed 2 -form ω on a manifold $\mathscr{M}$ is called a symplectic form, and the pair $(\mathscr{M}, \omega)$ is called a symplectic manifold.

Since a symplectic form ω is non-degenerate, a symplectic manifold $\mathscr{M}$ is necessarily even-dimensional, $\dim \mathscr{M} = 2n$. The nowhere vanishing $2n$-form ω^n defines a canonical orientation on $\mathscr{M}$, and as in the case $\mathscr{M} = T^*M$, $\frac{\omega^n}{n!}$ is called Liouville's volume form. We also have the general notion of a Lagrangian submanifold.

Definition. A submanifold $\mathscr{L}$ of a symplectic manifold $(\mathscr{M}, \omega)$ is called a Lagrangian submanifold, if $\dim \mathscr{L} = \frac{1}{2} \dim \mathscr{M}$ and the restriction of the symplectic form ω to $\mathscr{L}$ is 0 .

Symplectic manifolds form a category. A morphism between $(\mathscr{M}_1, \omega_1)$ and $(\mathscr{M}_2, \omega_2)$, also called a symplectomorphism, is a mapping $f : \mathscr{M}_1 \to \mathscr{M}_2$ such that $\omega_1 = f^*(\omega_2)$. When $\mathscr{M}_1 = \mathscr{M}_2$ and $\omega_1 = \omega_2$, the notion of a symplectomorphism generalizes the notion of a canonical transformation. The direct product of symplectic manifolds $(\mathscr{M}_1, \omega_1)$ and $(\mathscr{M}_2, \omega_2)$ is a symplectic manifold

$$(\mathscr{M}_1 \times \mathscr{M}_2, \pi_1^*(\omega_1) + \pi_2^*(\omega_2))$$

where π_1 and π_2 are, respectively, projections of $\mathscr{M}_1 \times \mathscr{M}_2$ onto the first and second factors in the Cartesian product.

Besides cotangent bundles, another important class of symplectic manifolds is given by Khler manifolds [17]. Recall that a complex manifold $\mathscr{M}$ is a Khler manifold if it carries the Hermitian metric whose imaginary part is a closed (1,1)-form. In local complex coordinates $\boldsymbol{z} = (z^1, ..., z^n)$ on $\mathscr{M}$ the Hermitian metric is written as

$$h = \sum_{\alpha,\beta=1}^{n} h_{\alpha\bar{\beta}}(\boldsymbol{z}, \overline{\boldsymbol{z}}) dz^\alpha \otimes d\bar{z}^\beta.$$

Correspondingly,

$$g = \operatorname{Re} h = \frac{1}{2} \sum_{\alpha,\beta=1}^{n} h_{\alpha\bar{\beta}}(\boldsymbol{z}, \overline{\boldsymbol{z}}) \left(dz^\alpha \otimes d\bar{z}^\beta + d\bar{z}^\beta \otimes dz^\alpha \right)$$

is the Riemannian metric on $\mathscr{M}$ and

$$\omega = -\operatorname{Im} h = \frac{i}{2} \sum_{\alpha,\beta=1}^{n} h_{\alpha\bar{\beta}}(\boldsymbol{z}, \overline{\boldsymbol{z}}) dz^\alpha \wedge d\bar{z}^\beta$$

is the symplectic form on $\mathscr{M}$ (considered as a $2n$-dimensional real manifold).
The simplest compact Khler manifold is $\mathbb{C}P^1 \simeq S^2$ with the symplectic form given by the area 2 -form of the Hermitian metric of Gaussian curvature 1 - the round metric on the 2 -sphere. In terms of the local coordinate z associated with the stereographic projection $\mathbb{C}P^1 \simeq \mathbb{C} \cup \{\infty\}$,

$$\omega = 2i \frac{dz \wedge d\bar{z}}{(1 + |z|^2)^2}$$

Similarly, the natural symplectic form on the complex projective space $\mathbb{C}P^n$ is the symplectic form of the Fubini-Study metric. By pull-back, it defines symplectic forms on complex projective varieties.

The simplest non-compact Khler manifold is the n-dimensional complex vector space $\mathbb{C}^n$ with the standard Hermitian metric. In complex coordinates $\boldsymbol{z} = (z^1, ..., z^n)$ on $\mathbb{C}^n$ it is given by

$$h = d\boldsymbol{z} \otimes d\overline{\boldsymbol{z}} = \sum_{\alpha=1}^{n} dz^\alpha \otimes d\bar{z}^\alpha.$$

In terms of real coordinates $(\boldsymbol{x}, \boldsymbol{y}) = (x^1, ..., x^n, y^1, ..., y^n)$ on $\mathbb{R}^{2n} \simeq \mathbb{C}^n$, where $\boldsymbol{z} = \boldsymbol{x} + i\boldsymbol{y}$, the corresponding symplectic form $\omega = -\operatorname{Im} h$ has the canonical form

$$\omega = \frac{i}{2} d\boldsymbol{z} \wedge d\overline{\boldsymbol{z}} = \sum_{\alpha=1}^{n} dx^\alpha \wedge dy^\alpha = d\boldsymbol{x} \wedge d\boldsymbol{y}$$

[017] Needless to say, not every symplectic manifold admits a complex structure, not to mention a Khler structure.

This example naturally leads to the following definition.

Definition. A symplectic vector space is a pair (V, ω), where V is a vector space over $\mathbb{R}$ and ω is a non-degenerate, skew-symmetric bilinear form on V.

It follows from basic linear algebra that every symplectic vector space V has a symplectic basis - a basis $e^1, ..., e^n, f_1, ..., f_n$ of V, where $2n = \dim V$, such that

$$\omega\left(e^i, e^j\right) = \omega\left(f_i, f_j\right) = 0 \quad \text{and} \quad \omega\left(e^i, f_j\right) = \delta^i_j, \quad i, j = 1, ..., n.$$

In coordinates $(\boldsymbol{p}, \boldsymbol{q}) = (p_1, ..., p_n, q^1, ..., q^n)$ corresponding to this basis, $V \simeq \mathbb{R}^{2n}$ and

$$\omega = d\boldsymbol{p} \wedge d\boldsymbol{q} = \sum_{i=1}^{n} dp_i \wedge dq^i$$

Thus every symplectic vector space is isomorphic to a direct product of the phase planes $\mathbb{R}^2$ with the canonical symplectic form $dp \wedge dq$. Introducing complex coordinates $\boldsymbol{z} = \boldsymbol{p} + i\boldsymbol{q}$, we get the isomorphism $V \simeq \mathbb{C}^n$, so that every symplectic vector space admits a Khler structure.

It is a basic fact of symplectic geometry that every symplectic manifold is locally isomorphic to a symplectic vector space.

Theorem 2.11 (Darboux' theorem). Let $(\mathscr{M}, \omega)$ be a $2n$-dimensional symplectic manifold. For every point $x \in \mathscr{M}$ there is a neighborhood U of x with local coordinates $(\boldsymbol{p}, \boldsymbol{q}) = (p_1, ..., p_n, q^1, ..., q^n)$ such that on U

$$\omega = d\boldsymbol{p} \wedge d\boldsymbol{q} = \sum_{i=1}^{n} dp_i \wedge dq^i$$

Coordinates $\boldsymbol{p}, \boldsymbol{q}$ are called canonical coordinates (Darboux coordinates). The proof proceeds by induction on n with the two main steps stated as Problems 2.13 and 2.14.

A non-degenerate 2-form ω for every $x \in \mathscr{M}$ defines an isomorphism $J : T^*_x\mathscr{M} \to T_x\mathscr{M}$ by

$$\omega\left(u_1, u_2\right) = J^{-1}\left(u_2\right)\left(u_1\right), u_1, u_2 \in T_x\mathscr{M}.$$

Explicitly, for every $X \in \mathrm{Vect}(\mathscr{M})$ and $\vartheta \in \mathcal{A}^1(\mathscr{M})$ we have

$$\omega(X, J(\vartheta)) = \vartheta(X) \quad \text{and} \quad J^{-1}(X) = -i_X(\omega)$$

(cf. Section 2.1). In local coordinates $\boldsymbol{x} = (x^1, ..., x^{2n})$ for the coordinate chart (U, φ) on $\mathscr{M}$, the 2 -form ω is given by

$$\omega = \frac{1}{2} \sum_{i,j=1}^{2n} \omega_{ij}(\boldsymbol{x}) dx^i \wedge dx^j,$$

where $\{\omega_{ij}(\boldsymbol{x})\}_{i,j=1}^{2n}$ is a non-degenerate, skew-symmetric matrix-valued function on $\varphi(U)$. Denoting the inverse matrix by $\{\omega^{ij}(\boldsymbol{x})\}_{i,j=1}^{2n}$, we have

$$J\left(dx^i\right) = -\sum_{j=1}^{2n} \omega^{ij}(\boldsymbol{x}) \frac{\partial}{\partial x^j}, \quad i = 1, ..., 2n$$

Definition. A Hamiltonian system is a pair consisting of a symplectic manifold $(\mathscr{M}, \omega)$, called a phase space, and a smooth real-valued function H on $\mathscr{M}$, called a Hamiltonian. The motion of points on the phase space is described by the vector field

$$X_H = J(dH)$$

called a Hamiltonian vector field.
The trajectories of a Hamiltonian system $((\mathscr{M},\omega),H)$ are the integral curves of a Hamiltonian vector field X_H on $\mathscr{M}$. In canonical coordinates $(\boldsymbol{p},\boldsymbol{q})$ they are described by the canonical Hamilton's equations (2.1),

$$\dot{\boldsymbol{p}}=-\frac{\partial H}{\partial \boldsymbol{q}},\quad \dot{\boldsymbol{q}}=\frac{\partial H}{\partial \boldsymbol{p}}$$

Suppose now that the Hamiltonian vector field X_H on $\mathscr{M}$ is complete. The Hamiltonian phase flow on $\mathscr{M}$ associated with a Hamiltonian H is a oneparameter group $\{g_t\}_{t\in\mathbb{R}}$ of diffeomorphisms of $\mathscr{M}$ generated by X_H. The following statement generalizes Theorem 2.1.

Theorem 2.12. The Hamiltonian phase flow preserves the symplectic form.
Proof. It is sufficient to show that $\mathcal{L}_{X_H}\omega=0$. Using Cartan's formula

$$\mathcal{L}_X=i_X\circ d+d\circ i_X$$

and $d\omega=0$, we get for every $X\in \mathrm{Vect}(\mathscr{M})$,

$$\mathcal{L}_X\omega=(d\circ i_X)(\omega)$$

Since $i_X(\omega)(Y)=\omega(X,Y)$, we have for $X=X_H$ and every $Y\in\mathrm{Vect}(\mathscr{M})$ that

$$i_{X_H}(\omega)(Y)=\omega(J(dH),Y)=-dH(Y).$$

Thus $i_{X_H}(\omega)=-dH$, and the statement follows from $d^2=0$.
Corollary 2.13. A vector field X on $\mathscr{M}$ is a Hamiltonian vector field if and only if the 1 -form $i_X(\omega)$ is exact.

Definition. A vector field X on a symplectic manifold $(\mathscr{M},\omega)$ is called a symplectic vector field if the 1 -form $i_X(\omega)$ is closed, which is equivalent to $\mathscr{L}_X\omega=0$.

The commutative algebra $C^\infty(\mathscr{M})$, with a multiplication given by the point-wise product of functions, is called the algebra of classical observables. Assuming that the Hamiltonian phase flow g_t exists for all times, the time evolution of every observable $f\in C^\infty(\mathscr{M})$ is given by

$$f_t(x)=f\left(g_t(x)\right),\quad x\in\mathscr{M},$$

and is described by the differential equation

$$\frac{df_t}{dt}=X_H\left(f_t\right)$$

- Hamilton's equation for classical observables. Hamilton's equations for observables on $\mathscr{M}$ have the same form as Hamilton's equations on $\mathscr{M}=T^*M$, considered in Section 2.3. Since

$$X_H(f)=df\left(X_H\right)=\omega\left(X_H,J(df)\right)=\omega\left(X_H,X_f\right),$$

we have the following.

Definition. A Poisson bracket on the algebra $C^\infty(\mathscr{M})$ of classical observables on a symplectic manifold $(\mathscr{M},\omega)$ is a bilinear mapping $\{,\}:C^\infty(\mathscr{M})\times C^\infty(\mathscr{M})\to C^\infty(\mathscr{M})$, defined by

$$\{f,g\}=\omega\left(X_f,X_g\right),\quad f,g\in C^\infty(\mathscr{M}).$$

Now Hamilton's equation takes the concise form

$$\frac{df}{dt} = \{H, f\}, \tag{2.12}$$

understood as a differential equation for a family of functions f_t on $\mathscr{M}$ with the initial condition $f_t|_{t=0} = f$. In local coordinates $\boldsymbol{x} = (x^1, ..., x^{2n})$ on $\mathscr{M}$,

$$\{f, g\}(\boldsymbol{x}) = -\sum_{i,j=1}^{2n} \omega^{ij}(\boldsymbol{x}) \frac{\partial f(\boldsymbol{x})}{\partial x^i} \frac{\partial g(\boldsymbol{x})}{\partial x^j}.$$

Theorem 2.14. The Poisson bracket $\{,\}$ *on a symplectic manifold* $(\mathscr{M}, \omega)$ is skew-symmetric and satisfies Leibniz rule and the Jacobi identity.

Proof. The first two properties are obvious. It follows from the definition of a Poisson bracket and the formula

$$[X_f, X_g](h) = (X_g X_f - X_f X_g)(h) = \{g, \{f, h\}\} - \{f, \{g, h\}\}$$

that the Jacobi identity is equivalent to the property

$$[X_f, X_g] = X_{\{f,g\}} \tag{2.13}$$

Let X and Y be symplectic vector fields. Using Cartan's formulas we get

$$\begin{aligned} i_{[X,Y]}(\omega) &= \mathcal{L}_X (i_Y(\omega)) - i_Y (\mathcal{L}_X(\omega)) \\ &= d (i_X \circ i_Y(\omega)) + i_X d (i_Y(\omega)) \\ &= d(\omega(Y, X)) = i_Z(\omega) \end{aligned}$$

where Z is a Hamiltonian vector field corresponding to $\omega(X, Y) \in C^\infty(\mathscr{M})$. Since the 2-form ω is non-degenerate, this implies $[X, Y] = Z$, so that setting $X = X_f, Y = X_g$ and using $\{f, g\} = \omega(X_f, X_g)$, we get (2.13).

From (2.13) we immediately get the following result.

Corollary 2.15. The subspace $\mathrm{Ham}(\mathscr{M})$ of Hamiltonian vector fields on $\mathscr{M}$ is a Lie subalgebra of $\mathrm{Vect}(\mathscr{M})$. The mapping $C^\infty(\mathscr{M}) \to \mathrm{Ham}(\mathscr{M})$, given by $f \mapsto X_f$, is a Lie algebra homomorphism with the kernel consisting of locally constant functions on $\mathscr{M}$.

As in the case $\mathscr{M} = T^*M$ (see Section 2.4), an observable I - a function on the phase space $\mathscr{M}$ - is called an integral of motion (first integral) for the Hamiltonian system $((\mathscr{M}, \omega), H)$ if it is constant along the Hamiltonian phase flow. According to (2.12), this is equivalent to the condition

$$\{H, I\} = 0. \tag{2.14}$$

It is said that the observables H and I are in involution (Poisson commute). From the Jacobi identity for the Poisson bracket we get the following result.

Corollary 2.16 (Poisson's theorem). The Poisson bracket of two integrals of motion is an integral of motion.

Proof. If $\{H, I_1\} = \{H, I_2\} = 0$, then

$$\{H, \{I_1, I_2\}\} = \{\{H, I_1\}, I_2\} - \{\{H, I_2\}, I_1\} = 0.$$

It follows from Poisson's theorem that integrals of motion form a Lie algebra and, by (2.13), corresponding Hamiltonian vector fields form a Lie subalgebra in $\mathrm{Vect}(\mathscr{M})$. Since $\{I, H\} = dH(X_I) = 0$, the vector fields X_I are tangent to submanifolds $\mathscr{M}_E = \{x \in \mathscr{M} : H(x) = E\}$ - the level sets of the Hamiltonian H. This defines a Lie algebra of integrals of motion for the Hamiltonian system $((\mathscr{M}, \omega), H)$ at the level set $\mathscr{M}_E$.

Let G be a finite-dimensional Lie group that acts on a connected symplectic manifold $(\mathscr{M}, \omega)$ by symplectomorphisms. The Lie algebra $\mathfrak{g}$ of G acts on $\mathscr{M}$ by vector fields

$$X_\xi(f)(x) = \left.\frac{d}{ds}\right|_{s=0} f\left(e^{-s\xi} \cdot x\right)$$

and the linear mapping $\mathfrak{g} \ni \xi \mapsto X_\xi \in \mathrm{Vect}(\mathscr{M})$ is a homomorphism of Lie algebras,

$$[X_\xi, X_\eta] = X_{[\xi,\eta]}, \quad \xi, \eta \in \mathfrak{g}.$$

The G-action is called a Hamiltonian action if X_ξ are Hamiltonian vector fields, i.e., for every $\xi \in \mathfrak{g}$ there is $\Phi_\xi \in C^\infty(\mathscr{M})$, defined up to an additive constant, such that $X_\xi = X_{\Phi_\xi} = J\,(d\Phi_\xi)$. It is called a Poisson action if there is a choice of functions Φ_ξ such that the linear mapping $\Phi : \mathfrak{g} \to C^\infty(\mathscr{M})$ is a homomorphism of Lie algebras,

$$\{\Phi_\xi, \Phi_\eta\} = \Phi_{[\xi,\eta]}, \quad \xi, \eta \in \mathfrak{g}. \tag{2.15}$$

Definition. A Lie group G is a symmetry group of the Hamiltonian system $((\mathscr{M}, \omega), H)$ if there is a Hamiltonian action of G on $\mathscr{M}$ such that

$$H(g \cdot x) = H(x), \quad g \in G, x \in \mathscr{M}.$$

Theorem 2.17 (Noether theorem with symmetries). If G is a symmetry group of the Hamiltonian system $((\mathscr{M}, \omega), H)$, then the functions $\Phi_\xi, \xi \in \mathfrak{g}$, are the integrals of motion. If the action of G is Poisson, the integrals of motion satisfy (2.15).

Proof. By definition of the Hamiltonian action, for every $\xi \in \mathfrak{g}$,

$$0 = X_\xi(H) = X_{\Phi_\xi}(H) = \{\Phi_\xi, H\}$$

Corollary 2.18. Let (M, L) be a Lagrangian system such that the Legendre transform $\tau_L : TM \to T^*M$ is a diffeomorphism. Then if a Lie group G is a symmetry of (M, L), then G is a symmetry group of the corresponding Hamiltonian system $\left((T^*M, \omega), H = E_L \circ \tau_L^{-1}\right)$, and the corresponding G action on T^*M is Poisson. In particular, $\Phi_\xi = -I_\xi \circ \tau_L^{-1}$, where I_ξ are Noether integrals of motion for the one-parameter subgroups of G generated by $\xi \in \mathfrak{g}$.

Proof. Let X be the vector field associated with the one-parameter subgroup $\left\{e^{s\xi}\right\}_{s\in\mathbb{R}}$ of diffeomorphisms of M, used in Theorem 1.3, and let X' be its lift to TM. We have [18]

$$X_\xi = -\left(\tau_L\right)_* (X') \tag{2.16}$$

and it follows from (1.16) that $\Phi_\xi = i_{X_\xi}(\theta) = \theta\,(X_\xi)$, where θ is the canonical Liouville 1-form on T^*M. From Cartan's formula and (1.17) we get

$$d\Phi_\xi = d\left(i_{X_\xi}(\theta)\right) = -i_{X_\xi}(d\theta) + \mathcal{L}_{X_\xi}(\theta) = -i_{X_\xi}(\omega)$$

so that

$$J\,(d\Phi_\xi) = -J\left(i_{X_\xi}(\omega)\right) = X_\xi$$

and the G-action is Hamiltonian. Using (1.17) and another Cartan's formula, we obtain

$$\begin{aligned}\Phi_{[\xi,\eta]} = i_{\left[X_\xi, X_\eta\right]}(\theta) &= \mathcal{L}_{X_\xi}\left(i_{X_\eta}(\theta)\right) + i_{X_\eta}\left(\mathcal{L}_{X_\xi}(\theta)\right) \\ &= X_\xi\left(\Phi_\eta\right) = \left\{\Phi_\xi, \Phi_\eta\right\}.\end{aligned}$$

[018] The negative sign reflects the difference in definitions of X and X_ξ.

Example 2.1. The Lagrangian

$$L = \frac{1}{2}m\dot{\boldsymbol{r}}^2 - V(r)$$

for a particle in $\mathbb{R}^3$ moving in a central field (see Section 1.6) is invariant with respect to the action of the group SO(3) of orthogonal transformations of the Euclidean space $\mathbb{R}^3$. Let u_1, u_2, u_3 be a basis for the Lie algebra $\mathfrak{so}(3)$ corresponding to the rotations with the axes given by the vectors of the standard basis e_1, e_2, e_3 for $\mathbb{R}^3$ (see Example 1.10 in Section 1.4). These generators satisfy the commutation relations

$$[u_i, u_j] = \varepsilon_{ijk}u_k$$

where $i, j, k = 1, 2, 3$, and ε_{ijk} is a totally anti-symmetric tensor, $\varepsilon_{123} = 1$. Corresponding Noether integrals of motion are given by $\Phi_{u_i} = -M_i$, where

$$\begin{aligned} M_1 &= (\boldsymbol{r} \times \boldsymbol{p})_1 = r_2p_3 - r_3p_2, \\ M_2 &= (\boldsymbol{r} \times \boldsymbol{p})_2 = r_3p_1 - r_1p_3, \\ M_3 &= (\boldsymbol{r} \times \boldsymbol{p})_3 = r_1p_2 - r_2p_1 \end{aligned}$$

are components of the angular momentum vector $\boldsymbol{M} = \boldsymbol{r} \times \boldsymbol{p}$. (Here it is convenient to lower the indices of the coordinates r_i by the Euclidean metric on $\mathbb{R}^3$.) For the Hamiltonian

$$H = \frac{\boldsymbol{p}^2}{2m} + V(r)$$

we have

$$\{H, M_i\} = 0$$

According to Theorem 2.17 and Corollary 2.18, Poisson brackets of the components of the angular momentum satisfy

$$\{M_i, M_j\} = -\varepsilon_{ijk}M_k,$$

which is also easy to verify directly using (2.6),

$$\{f, g\}(\boldsymbol{p}, \boldsymbol{r}) = \frac{\partial f}{\partial \boldsymbol{p}}\frac{\partial g}{\partial \boldsymbol{r}} - \frac{\partial f}{\partial \boldsymbol{r}}\frac{\partial g}{\partial \boldsymbol{p}}$$

Example 2.2 (Kepler's problem). For every $\alpha \in \mathbb{R}$ the Lagrangian system on $\mathbb{R}^3$ with

$$L = \frac{1}{2}m\dot{r}^2 + \frac{\alpha}{r}$$

has three extra integrals of motion - the components W_1, W_2, W_3 of the Laplace-Runge-Lenz vector, given by

$$\boldsymbol{W} = \frac{\boldsymbol{p}}{m} \times \boldsymbol{M} - \frac{\alpha \boldsymbol{r}}{r}$$

(see Section 1.6). Using Poisson brackets from the previous example, together with $\{r_i, M_j\} = -\varepsilon_{ijk}r_k$ and $\{p_i, M_j\} = -\varepsilon_{ijk}p_k$, we get by a straightforward computation,

$$\{W_i, M_j\} = -\varepsilon_{ijk}W_k \quad \text{and} \quad \{W_i, W_j\} = \frac{2H}{m}\varepsilon_{ijk}M_k$$

where $H = \frac{\boldsymbol{p}^2}{2m} - \frac{\alpha}{r}$ is the Hamiltonian of Kepler's problem.
The Hamiltonian system $((\mathscr{M}, \omega), H), \dim \mathscr{M} = 2n$, is called completely integrable if it has

n independent integrals of motion $F_1 = H, ..., F_n$ in involution. The former condition means that $dF_1(x), ..., dF_n(x) \in T_x^*\mathscr{M}$ are linearly independent for almost all $x \in \mathscr{M}$. Hamiltonian systems with one degree of freedom such that dH has only finitely many zeros are completely integrable. Complete separation of variables in the Hamilton-Jacobi equation (see Section 2.5) provides other examples of completely integrable Hamiltonian systems.

Let $((\mathscr{M}, \omega), H)$ be a completely integrable Hamiltonian system. Suppose that the level set $\mathscr{M}_f = \{x \in \mathscr{M} : F_1(x) = f_1, ..., F_n(x) = f_n\}$ is compact and tangent vectors $JdF_1, ..., JdF_n$ are linearly independent for all $x \in \mathscr{M}_f$. Then by the Liouville-Arnold theorem, in a neighborhood of $\mathscr{M}_f$ there exist so-called action-angle variables: coordinates $\boldsymbol{I} = (I_1, ..., I_n) \in \mathbb{R}_+^n = (\mathbb{R}_{>0})^n$ and $\varphi = (\varphi_1, ..., \varphi_n) \in T^n = (\mathbb{R}/2\pi\mathbb{Z})^n$ such that $\omega = d\boldsymbol{I} \wedge d\varphi$ and $H = H(I_1, ..., I_n)$. According to Hamilton's equations,

$$\dot{I}_i = 0 \quad \text{and} \quad \dot{\varphi}_i = \omega_i = \frac{\partial H}{\partial I_i}, \quad i = 1, ..., n$$

so that action variables are constants, and angle variables change uniformly, $\varphi_i(t) = \varphi_i(0) + \omega_i t, i = 1, ..., n$. The classical motion is almost-periodic with the frequencies $\omega_1, ..., \omega_n$.

Problem 2.10. Show that a symplectic manifold $(\mathscr{M}, \omega)$ admits an almost complex structure: a bundle map $\mathscr{J} : T\mathscr{M} \to T\mathscr{M}$ such that $\mathscr{J}^2 = -\mathrm{id}$.

Problem 2.11. Give an example of a symplectic manifold which admits a complex structure but not a Khler structure.

Problem 2.12 (Coadjont orbits). Let G be a finite-dimensional Lie group, let $\mathfrak{g}$ be its Lie algebra, and let $\mathfrak{g}^*$ be the dual vector space to $\mathfrak{g}$. For $u \in \mathfrak{g}^*$ let $\mathscr{M} = \mathcal{O}_u$ be the orbit of u under the coadjoint action of G on $\mathfrak{g}^*$. Show that the formula

$$\omega(u_1, u_2) = u([x_1, x_2]),$$

where $u_1 = \mathrm{ad}^* x_1(u), u_2 = \mathrm{ad}^* x_2(u) \in \mathcal{O}_u$, and ad* stands for the coadjoint action of a Lie algebra $\mathfrak{g}$ on $\mathfrak{g}^*$, gives rise to a well-defined 2 -form on $\mathscr{M}$, which is closed and non-degenerate. (The 2 -form ω is called the Kirillov-Kostant symplectic form.)

Problem 2.13. Let $(\mathscr{M}, \omega)$ be a symplectic manifold. For $x \in \mathscr{M}$ choose a function q^1 on $\mathscr{M}$ such that $q^1(x) = 0$ and dq^1 does not vanish at x, and set $X = -X_{q^1}$. Show that there is a neighborhood U of $x \in \mathscr{M}$ and a function p_1 on U such that $X(q^1) = 1$ on U, and there exist coordinates $p_1, q^1, z^1, ..., z^{2n-2}$ on U such that

$$X = \frac{\partial}{\partial p_1} \quad \text{and} \quad Y = X_{p_1} = \frac{\partial}{\partial q^1}$$

Problem 2.14. Continuing Problem 2.13, show that the 2 -form $\omega - dp_1 \wedge dq^1$ on U depends only on coordinates $z^1, ..., z^{2n-2}$ and is non-degenerate.

Problem 2.15. Do the computation in Example 2.2 and show that the Lie algebra of the integrals $M_1, M_2, M_3, W_1, W_2, W_3$ in Kepler's problem at $H(\boldsymbol{p}, \boldsymbol{r}) = E$ is isomorphic to the Lie algebra $\mathfrak{so}(4)$, if $E < 0$, to the Euclidean Lie algebra $\mathfrak{e}(3)$, if $E = 0$, and to the Lie algebra $\mathfrak{so}(1, 3)$, if $E > 0$.

Problem 2.16. Find the action-angle variables for a particle with one degree of freedom, when the potential $V(x)$ is a convex function on $\mathbb{R}$ satisfying $\lim_{|x|\to\infty} V(x) = \infty$. (Hint: Define $I = \oint p dx$, where integration goes over the closed orbit with $H(p, x) = E$.)

Problem 2.17. Show that a Hamiltonian system describing a particle in $\mathbb{R}^3$ moving in a central field is completely integrable, and find the action-angle variables.

Problem 2.18 (Symplectic quotients). For a Poisson action of a Lie group G on a symplectic manifold $(\mathscr{M}, \omega)$, define the moment map $P : \mathscr{M} \to \mathfrak{g}^*$ by

$$P(x)(\xi) = \Phi_\xi(x), \xi \in \mathfrak{g}, x \in \mathscr{M},$$

where $\mathfrak{g}$ is the Lie algebra of G. For every $p \in \mathfrak{g}^*$ such that a stabilizer G_p of p acts freely and properly on $\mathscr{M}_p = P^{-1}(p)$ (such p is called the regular value of the moment map), the quotient $M_p = G_p \backslash \mathscr{M}_p$ is called a reduced phase space. Show that M_p is a symplectic manifold with the symplectic form uniquely characterized by the condition that its pull-back to $\mathscr{M}_p$ coincides with the restriction to $\mathscr{M}_p$ of the symplectic form ω.

2.7. Poisson manifolds.

The notion of a Poisson manifold generalizes the notion of a symplectic manifold.

Definition. A Poisson manifold is a manifold $\mathscr{M}$ equipped with a Poisson structure - a skew-symmetric bilinear mapping

$$\{,\} : C^\infty(\mathscr{M}) \times C^\infty(\mathscr{M}) \to C^\infty(\mathscr{M})$$

which satisfies the Leibniz rule and Jacobi identity.

Equivalently, $\mathscr{M}$ is a Poisson manifold if the algebra $\mathcal{A} = C^\infty(\mathscr{M})$ of classical observables is a Poisson algebra - a Lie algebra such that the Lie bracket is a bi-derivation with respect to the multiplication in $\mathcal{A}$ (a pointwise product of functions). It follows from the derivation property that in local coordinates $\boldsymbol{x} = \left(x^1, ..., x^N\right)$ on $\mathscr{M}$, the Poisson bracket has the form

$$\{f, g\}(\boldsymbol{x}) = \sum_{i,j=1}^{N} \eta^{ij}(\boldsymbol{x}) \frac{\partial f(\boldsymbol{x})}{\partial x^i} \frac{\partial g(\boldsymbol{x})}{\partial x^j}.$$

The 2-tensor $\eta^{ij}(\boldsymbol{x})$, called a Poisson tensor, defines a global section η of the vector bundle $T\mathscr{M} \wedge T\mathscr{M}$ over $\mathscr{M}$.

The evolution of classical observables on a Poisson manifold is given by Hamilton's equations, which have the same form as (2.12),

$$\frac{df}{dt} = X_H(f) = \{H, f\}.$$

The phase flow g_t for a complete Hamiltonian vector field $X_H = \{H, \cdot\}$ defines the evolution operator $U_t : \mathcal{A} \to \mathcal{A}$ by

$$U_t(f)(x) = f\left(g_t(x)\right), f \in \mathcal{A}.$$

Theorem 2.19. Suppose that every Hamiltonian vector field on a Poisson manifold $(\mathscr{M}, \{\},)is complete. Then for every H \in \mathcal{A}$, the corresponding evolution operator U_t is an automorphism of the Poisson algebra $\mathcal{A}$, i.e.,

$$U_t(\{f, g\}) = \{U_t(f), U_t(g)\} \quad \text{for all} \quad f, g \in \mathcal{A}. \tag{2.17}$$

Conversely, if a skew-symmetric bilinear mapping $\{\} :, C^\infty(\mathscr{M}) \times C^\infty(\mathscr{M}) \to C^\infty(\mathscr{M})$ is such that $X_H = \{H, \cdot\}$ are complete vector fields for all $H \in \mathcal{A}$, and corresponding evolution operators U_t satisfy (2.17), then $(\mathscr{M}, \{\},$ is a Poisson manifold.

Proof. Let $f_t = U_t(f), g_t = U_t(g)$, and [19] $h_t = U_t(\{f, g\})$. By definition,

$$\frac{d}{dt}\{f_t, g_t\} = \{\{H, f_t\}, g_t\} + \{f_t, \{H, g_t\}\} \quad \text{and} \quad \frac{dh_t}{dt} = \{H, h_t\}.$$

If $(\mathscr{M}, \{\},) is a Poisson manifold, then it follows from the Jacobi identity$ that

$$\{\{H, f_t\}, g_t\} + \{f_t, \{H, g_t\}\} = \{H, \{f_t, g_t\}\},$$

so that h_t and $\{f_t, g_t\}$ satisfy the same differential equation (2.12). Since these functions coincide at $t = 0$, (2.17) follows from the uniqueness theorem for the ordinary differential equations.

Conversely, we get the Jacobi identity for the functions f, g, and H by differentiating (2.17) with respect to t at $t = 0$.

Corollary 2.20. A global section η of $T\mathscr{M} \wedge T\mathscr{M}$ is a Poisson tensor if and only if

$$\mathcal{L}_{X_f}\eta = 0 \quad \text{for all} \quad f \in \mathcal{A}.$$

Definition. The center of a Poisson algebra $\mathcal{A}$ is

$$\mathcal{Z}(\mathcal{A}) = \{f \in \mathcal{A} : \{f, g\} = 0 \quad \text{for all } g \in \mathcal{A}\}$$

A Poisson manifold $(\mathscr{M}, \{,\})is called non-degenerate if the center of a$ Poisson algebra of classical observables $\mathcal{A} = C^\infty(\mathscr{M})$ consists only of locally constant functions ($\mathcal{Z}(\mathcal{A}) = \mathbb{R}$ for connected $\mathscr{M}$).

Equivalently, a Poisson manifold $(\mathscr{M}, \{\},)is non-degenerate if the Pois$ - son tensor η is non-degenerate everywhere on $\mathscr{M}$, so that $\mathscr{M}$ is necessarily an even-dimensional manifold. A non-degenerate Poisson tensor for every $x \in \mathscr{M}$ defines an isomorphism $J : T_x^*\mathscr{M} \to T_x\mathscr{M}$ by

$$\eta(u_1, u_2) = u_2(J(u_1)), u_1, u_2 \in T_x^*\mathscr{M}.$$

In local coordinates $\boldsymbol{x} = \left(x^1, ..., x^N\right)$ for the coordinate chart (U, φ) on $\mathscr{M}$, we have

$$J\left(dx^i\right) = \sum_{j=1}^{N} \eta^{ij}(\boldsymbol{x}) \frac{\partial}{\partial x^j}, \quad i = 1, ..., N$$

Poisson manifolds form a category. A morphism between $(\mathscr{M}_1, \{,\}_1)$ and $(\mathscr{M}_2, \{,\}_2)$ is a mapping $\varphi : \mathscr{M}_1 \to \mathscr{M}_2$ of smooth manifolds such that

$$\{f \circ \varphi, g \circ \varphi\}_1 = \{f, g\}_2 \circ \varphi \quad \text{for all } f, g \in C^\infty(\mathscr{M}_2)$$

A direct product of Poisson manifolds $(\mathscr{M}_1, \{,\}_1)$ and $(\mathscr{M}_2, \{,\}_2)$ is a Poisson manifold $(\mathscr{M}_1 \times \mathscr{M}_2, \{\},)$ defined by the property that natural projection maps $\pi_1 : \mathscr{M}_1 \times \mathscr{M}_2 \to \mathscr{M}_1$ and $\pi_2 : \mathscr{M}_1 \times \mathscr{M}_2 \to \mathscr{M}_2$ are Poisson mappings. For $f \in C^\infty(\mathscr{M}_1 \times \mathscr{M}_2)$ and $(x_1, x_2) \in \mathscr{M}_1 \times \mathscr{M}_2$ denote, respectively, by $f_{x_2}^{(1)}$ and $f_{x_1}^{(2)}$ restrictions of f to $\mathscr{M} \times \{x_2\}$ and $\{x_1\} \times \mathscr{M}_2$. Then for $f, g \in C^\infty(\mathscr{M}_1 \times \mathscr{M}_2)$,

$$\{f, g\}(x_1, x_2) = \left\{f_{x_2}^{(1)}, g_{x_2}^{(1)}\right\}_1(x_1) + \left\{f_{x_1}^{(2)}, g_{x_1}^{(2)}\right\}_2(x_2)$$

Non-degenerate Poisson manifolds form a subcategory of the category of Poisson manifolds.

Theorem 2.21. The category of symplectic manifolds is (anti-) isomorphic to the category of non-degenerate Poisson manifolds.

Proof. According to Theorem 2.14, every symplectic manifold carries a Poisson structure. Its non-degeneracy follows from the non-degeneracy of a symplectic form. Conversely, let $(\mathscr{M}, \{\},)be a non-degenerate Poisson$ manifold. Define the 2 -form ω on $\mathscr{M}$ by

$$\omega(X, Y) = J^{-1}(Y)(X), \quad X, Y \in \mathrm{Vect}(\mathscr{M})$$

where the isomorphism $J : T^*\mathscr{M} \to T\mathscr{M}$ is defined by the Poisson tensor η. In local coordinates $\boldsymbol{x} = \left(x^1, ..., x^N\right)$ on $\mathscr{M}$,

[019] Here g_t is not the phase flow!

$$\omega = -\sum_{1\leq i<j\leq N} \eta_{ij}(\boldsymbol{x}) dx^i \wedge dx^j$$

where $\{\eta_{ij}(\boldsymbol{x})\}_{i,j=1}^N$ is the inverse matrix to $\{\eta^{ij}(\boldsymbol{x})\}_{i,j=1}^N$. The 2 -form ω is skew-symmetric and non-degenerate. For every $f \in \mathcal{A}$ let $X_f = \{f, \cdot\}$ be the corresponding vector field on $\mathscr{M}$. The Jacobi identity for the Poisson bracket $\{,\} is equivalent to \mathcal{L}_{X_f}\eta = 0$ for every $f \in \mathcal{A}$, so that

$$\mathcal{L}_{X_f}\omega = 0.$$

Since $X_f = Jdf$, we have $\omega(X, Jdf) = df(X)$ for every $X \in \mathrm{Vect}(\mathscr{M})$, so that

$$\omega\left(X_f, X_g\right) = \{f, g\}.$$

By Cartan's formula,

$$\begin{aligned} d\omega(X,Y,Z) =& \frac{1}{3}\left(\mathcal{L}_X\omega(Y,Z) - \mathcal{L}_Y\omega(X,Z) + \mathcal{L}_Z\omega(X,Y)\right. \\ & \left. - \omega([X,Y],Z) + \omega([X,Z],Y) - \omega([Y,Z],X)\right), \end{aligned}$$

where $X, Y, Z \in \mathrm{Vect}(\mathscr{M})$. Now setting $X = X_f, Y = X_g, Z = X_h$, we get

$$\begin{aligned} d\omega\left(X_f, X_g, X_h\right) &= \frac{1}{3}\left(\omega\left(X_h, [X_f, X_g]\right) + \omega\left(X_f, [X_g, X_h]\right) + \omega\left(X_g, [X_h, X_f]\right)\right) \\ &= \frac{1}{3}\left(\omega\left(X_h, X_{\{f,g\}}\right) + \omega\left(X_f, X_{\{g,h\}}\right) + \omega\left(X_g, X_{\{h,f\}}\right)\right) \\ &= \frac{1}{3}(\{h,\{f,g\}\} + \{f,\{g,h\}\} + \{g,\{h,f\}\}) \\ &= 0. \end{aligned}$$

The exact 1 -forms $df, f \in \mathcal{A}$, generate the vector space of 1 -forms $\mathcal{A}^1(\mathscr{M})$ as a module over $\mathcal{A}$, so that Hamiltonian vector fields $X_f = Jdf$ generate the vector space $\mathrm{Vect}(\mathscr{M})$ as a module over $\mathcal{A}$. Thus $d\omega = 0$ and $(\mathscr{M}, \omega)$ is a symplectic manifold associated with the Poisson manifold $(\mathscr{M}, \{\},)$. It follows from the definitions that Poisson mappings of non-degenerate Poisson manifolds correspond to symplectomorphisms of associated symplectic manifolds.

Remark. One can also prove this theorem by a straightforward computation in local coordinates $\boldsymbol{x} = \left(x^1, ..., x^N\right)$ on $\mathscr{M}$. Just observe that the condition

$$\frac{\partial \eta_{ij}(\boldsymbol{x})}{\partial x^l} + \frac{\partial \eta_{jl}(\boldsymbol{x})}{\partial x^i} + \frac{\partial \eta_{li}(\boldsymbol{x})}{\partial x^j} = 0, \quad i,j,l = 1, ..., N$$

which is a coordinate form of $d\omega = 0$, follows from the condition

$$\sum_{j=1}^N \left(\eta^{ij}(\boldsymbol{x})\frac{\partial \eta^{kl}(\boldsymbol{x})}{\partial x^j} + \eta^{lj}(\boldsymbol{x})\frac{\partial \eta^{ik}(\boldsymbol{x})}{\partial x^j} + \eta^{kj}(\boldsymbol{x})\frac{\partial \eta^{li}(\boldsymbol{x})}{\partial x^j}\right) = 0$$

which is a coordinate form of the Jacobi identity, by multiplying it three times by the inverse matrix $\eta_{ij}(\boldsymbol{x})$ using

$$\sum_{p=1}^N \left(\eta^{ip}(\boldsymbol{x})\frac{\partial \eta_{pk}(\boldsymbol{x})}{\partial x^j} + \frac{\partial \eta^{ip}(\boldsymbol{x})}{\partial x^j}\eta_{pk}(\boldsymbol{x})\right) = 0.$$

Remark. Let $\mathscr{M} = T^*\mathbb{R}^n$ with the Poisson bracket $\{,\} given by the canon$ - ical symplectic form $\omega = d\boldsymbol{p} \wedge d\boldsymbol{q}$, where $(\boldsymbol{p}, \boldsymbol{q}) = (p_1, ..., p_n, q^1, ..., q^n)$ are coordinate functions on $T^*\mathbb{R}^n$. The non-degeneracy of the Poisson manifold $(T^*\mathbb{R}^n, \{\},)$ can be formulated as the property that the only observable $f \in C^\infty\left(T^*\mathbb{R}^n\right)$ satisfying

$$\{f, p_1\} = \cdots = \{f, p_n\} = 0, \quad \{f, q^1\} = \cdots = \{f, q^n\} = 0$$

is $f(\boldsymbol{p}, \boldsymbol{q}) = \text{const}$.

Problem 2.19 (Dual space to a Lie algebra). Let $\mathfrak{g}$ be a finite-dimensional Lie algebra with a Lie bracket $[,]$, and let $\mathfrak{g}^*$ be its dual space. For $f, g \in C^\infty(\mathfrak{g}^*)$ define

$$\{f, g\}(u) = u([df, dg]),$$

where $u \in \mathfrak{g}^*$ and $T_u^*\mathfrak{g}^* \simeq \mathfrak{g}$. Prove that $\{,\}$ *is a Poisson bracket.* (*It was introduced* by Sophus Lie and is called a linear, or Lie-Poisson bracket.) Show that this bracket is degenerate and determine the center of $\mathcal{A} = C^\infty(\mathfrak{g}^*)$.

Problem 2.20. A Poisson bracket $\{,\}$ *on* $\mathscr{M}$ restricts to a Poisson bracket $\{,\}_0$ on a submanifold $\mathscr{N}$ if the inclusion $\imath : \mathscr{N} \to \mathscr{M}$ is a Poisson mapping. Show that the Lie-Poisson bracket on $\mathfrak{g}^*$ restricts to a non-degenerate Poisson bracket on a coadjoint orbit, associated with the Kirillov-Kostant symplectic form.

Problem 2.21 (Lie-Poisson groups). A finite-dimensional Lie group is called a Lie-Poisson group if it has a structure of a Poisson manifold $(G, \{\},)$ *such that* the group multiplication $G \times G \to G$ is a Poisson mapping, where $G \times G$ is a direct product of Poisson manifolds. Using a basis $\partial_1, ..., \partial_n$ of left-invariant vector fields on G corresponding to a basis $x_1, ..., x_n$ of the Lie algebra $\mathfrak{g}$, the Poisson bracket $\{,\}$ *can be written as*

$$\{f_1, f_2\}(g) = \sum_{i,j=1}^{n} \eta^{ij}(g) \partial_i f_1 \partial_j f_2,$$

where the 2-tensor $\eta^{ij}(g)$ defines a mapping $\eta : G \to \Lambda^2\mathfrak{g}$ by $\eta(g) = \sum_{i,j=1}^n \eta^{ij}(g) x_i \otimes x_j$. Show that the bracket $\{,\}$ *equips* G with a Lie-Poisson structure if and only if the following conditions are satisfied: (i) for all $g \in G$,

$$\xi^{ijk}(g) = \sum_{l=1}^{n} \left(\eta^{il}(g) \partial_l \eta^{jk}(g) + \eta^{jl}(g) \partial_l \eta^{ki}(g) + \eta^{kl}(g) \partial_l \eta^{ij}(g) \right)$$
$$+ \sum_{l,p=1}^{n} \left(c_{lp}^i \eta^{pj}(g) \eta^{kl}(g) + c_{lp}^j \eta^{pk}(g) \eta^{il}(g) + c_{lp}^k \eta^{pi}(g) \eta^{jl}(g) \right) = 0$$

where $[x_i, x_j] = \sum_{k=1}^n c_{ij}^k x_k$; (ii) the mapping η is a group 1-cocycle with the adjoint action on $\Lambda^2\mathfrak{g}$, i.e., $\eta(g_1 g_2) = \mathrm{Ad}^{-1} g_2 \cdot \eta(g_1) + \eta(g_2), g_1, g_2 \in G$.

Problem 2.22. Show that the second condition in the previous problem trivially holds when η is a coboundary, $\eta(g) = -r + \mathrm{Ad}^{-1} g \cdot r$ for some $r = \sum_{i,j=1}^n r^{ij} x_i \otimes x_j \in \Lambda^2\mathfrak{g}$, and then the first condition is satisfied if and only if the element

$$\xi(r) = [r_{12}, r_{13} + r_{23}] + [r_{13}, r_{23}] \in \Lambda^3\mathfrak{g}$$

is invariant under the adjoint action of $\mathfrak{g}$ on $\Lambda^3\mathfrak{g}$. Here $r_{12} = \sum_{i,j=1}^n r^{ij} x_i \otimes x_j \otimes 1$, $r_{13} = \sum_{i,j=1}^n r^{ij} x_i \otimes 1 \otimes x_j$, and $r_{23} = \sum_{i,j=1}^n r^{ij} 1 \otimes x_i \otimes x_j$ are corresponding elements in the universal enveloping algebra $U\mathfrak{g}$ of a Lie algebra $\mathfrak{g}$. In particular, G is a Lie-Poisson group if $\xi(r) = 0$, which is called the classical Yang-Baxter equation.

Problem 2.23. Suppose that $r = \sum_{i,j=1}^n r^{ij} x_i \otimes x_j \in \Lambda^2\mathfrak{g}$ is such that the matrix $\{r^{ij}\}$ is non-degenerate, and let $\{r_{ij}\}$ be the inverse matrix. Show that r satisfies the classical Yang-Baxter equation if and only if the map $c : \Lambda^2\mathfrak{g} \to \mathbb{C}$, defined by $c(x, y) = \sum_{i,j=1}^n r_{ij} u^i v^j$, where $x = \sum_{i=1}^n u^i x_i, y = \sum_{i=1}^n v^i x_i$, is a non-degenerate Lie algebra 2-cocycle, i.e., it satisfies

$$c(x, [y, z]) + c(z, [x, y]) + c(y, [z, x]) = 0, \quad x, y, z \in \mathfrak{g}.$$

2.8. Hamilton's and Liouville's representations.

To complete the formulation of classical mechanics, we need to describe the process of measurement. In physics, by a measurement of a classical system one understands the result of a physical experiment which gives numerical values for classical observables. The experiment consists of creating certain conditions for the system, and it is always assumed that these conditions can be repeated over and over. The conditions of the experiment define a state of the system if repeating these conditions results in probability distributions for the values of all observables of the system.

Mathematically, a state μ on the algebra $\mathcal{A} = C^\infty(\mathscr{M})$ of classical observables on the phase space $\mathscr{M}$ is the assignment

$$\mathcal{A} \ni f \mapsto \mu_f \in \mathscr{P}(\mathbb{R}),$$

where $\mathscr{P}(\mathbb{R})$ is a set of probability measures on $\mathbb{R}$ - Borel measures on $\mathbb{R}$ such that the total measure of $\mathbb{R}$ is 1 . For every Borel subset $E \subseteq \mathbb{R}$ the quantity $0 \leq \mu_f(E) \leq 1$ is a probability that in the state μ the value of the observable f belongs to E. By definition, the expectation value of an observable f in the state μ is given by the Lebesgue-Stieltjes integral

$$\mathrm{E}_\mu(f) = \int_{-\infty}^{\infty} \lambda d\mu_f(\lambda)$$

where $\mu_f(\lambda) = \mu_f((-\infty, \lambda))$ is a distribution function of the measure $d\mu_f$. The correspondence $f \mapsto \mu_f$ should satisfy the following natural properties.

S1. $|\mathrm{E}_\mu(f)| < \infty$ for $f \in \mathcal{A}_0$ - the subalgebra of bounded observables.

S2. $\mathrm{E}_\mu(1) = 1$, where 1 is the unit in $\mathcal{A}$.

S3. For all $a, b \in \mathbb{R}$ and $f, g \in \mathcal{A}$,

$$\mathrm{E}_\mu(af + bg) = a\mathrm{E}_\mu(f) + b\mathrm{E}_\mu(g),$$

if both $\mathrm{E}_\mu(f)$ and $\mathrm{E}_\mu(g)$ exist.

S4. If $f_1 = \varphi \circ f_2$ with smooth $\varphi : \mathbb{R} \to \mathbb{R}$, then for every Borel subset $E \subseteq \mathbb{R}$,

$$\mu_{f_1}(E) = \mu_{f_2}\left(\varphi^{-1}(E)\right)$$

It follows from property **S4** and the definition of the Lebesgue-Stieltjes integral that

$$\mathrm{E}_\mu(\varphi(f)) = \int_{-\infty}^{\infty} \varphi(\lambda) d\mu_f(\lambda) \tag{2.18}$$

In particular, $\mathrm{E}_\mu\left(f^2\right) \geq 0$ for all $f \in \mathcal{A}$, so that the states define normalized, positive, linear functionals on the subalgebra $\mathcal{A}_0$.

Assuming that the functional E_μ extends to the space of bounded, piecewise continuous functions on $\mathscr{M}$, and satisfies (2.18) for measurable functions φ, one can recover the distribution function from the expectation values by the formula

$$\mu_f(\lambda) = \mathrm{E}_\mu(\theta(\lambda - f)),$$

where $\theta(x)$ is the Heavyside step function,

$$\theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x \leq 0 \end{cases}$$

Indeed, let χ be the characteristic function of the interval $(-\infty, \lambda) \subset \mathbb{R}$. Using (2.18) and the definition of the Lebesgue-Stieltjes integral we get

$$\mathrm{E}_\mu(\theta(\lambda - f)) = \int_{-\infty}^{\infty} \chi(s) d\mu_f(s) = \mu_f((-\infty, \lambda)) = \mu_f(\lambda)$$

Every probability measure $d\mu$ on $\mathscr{M}$ defines the state on $\mathcal{A}$ by assigning [20] to every observable f a probability measure $\mu_f = f_*(\mu)$ on $\mathbb{R}$ - a pushforward of the measure $d\mu$ on $\mathscr{M}$ by the mapping $f : \mathscr{M} \to \mathbb{R}$. It is defined by $\mu_f(E) = \mu\left(f^{-1}(E)\right)$ for every Borel subset $E \subseteq \mathbb{R}$, and has the distribution function

$$\mu_f(\lambda) = \mu\left(f^{-1}(-\infty, \lambda)\right) = \int_{\mathscr{M}_\lambda(f)} d\mu,$$

where $\mathscr{M}_\lambda(f) = \{x \in \mathscr{M} : f(x) < \lambda\}$. It follows from the Fubini theorem that

$$E_\mu(f) = \int_{-\infty}^{\infty} \lambda d\mu_f(\lambda) = \int_{\mathscr{M}} f d\mu \tag{2.19}$$

It turns out that probability measures on $\mathscr{M}$ are essentially the only examples of states. Namely, for a locally compact topological space $\mathscr{M}$ the Riesz-Markov theorem asserts that for every positive, linear functional l on the space $C_{\mathrm{c}}(\mathscr{M})$ of continuous functions on $\mathscr{M}$ with compact support, there is a unique regular Borel measure $d\mu$ on $\mathscr{M}$ such that

$$l(f) = \int_{\mathscr{M}} f d\mu \quad \text{for all} \quad f \in C_{\mathrm{c}}(\mathscr{M})$$

This leads to the following definition of states in classical mechanics.

Definition. The set of states $\mathcal{S}$ for a Hamiltonian system with the phase space $\mathscr{M}$ is the convex set $\mathscr{P}(\mathscr{M})$ of all probability measures on $\mathscr{M}$. The states corresponding to Dirac measures $d\mu_x$ supported at points $x \in \mathscr{M}$ are called pure states, and the phase space $\mathscr{M}$ is also called the space of states [21]. All other states are called mixed states. A process of measurement in classical mechanics is the correspondence

$$\mathcal{A} \times \mathcal{S} \ni (f, \mu) \mapsto \mu_f = f_*(\mu) \in \mathscr{P}(\mathbb{R})$$

which to every observable $f \in \mathcal{A}$ and state $\mu \in \mathcal{S}$ assigns a probability measure μ_f on $\mathbb{R}$ - a push-forward of the measure $d\mu$ on $\mathscr{M}$ by f. For every Borel subset $E \subseteq \mathbb{R}$ the quantity $0 \leq \mu_f(E) \leq 1$ is the probability that for a system in the state μ the result of a measurement of the observable f is in the set E. The expectation value of an observable f in a state μ is given by (2.19).

In physics, pure states are characterized by having the property that a measurement of every observable always gives a well-defined result. Mathematically this can be expressed as follows. Let

$$\sigma_\mu^2(f) = \mathrm{E}_\mu\left((f - \mathrm{E}_\mu(f))^2\right) = \mathrm{E}_\mu\left(f^2\right) - \mathrm{E}_\mu(f)^2 \geq 0$$

be the variance of the observable f in the state μ.

Lemma 2.1. Pure states are the only states in which every observable has zero variance.

Proof. It follows from the Cauchy-Bunyakovski-Schwarz inequality that $\sigma_\mu^2(f) = 0$ if only if f is constant on the support of a probability measure $d\mu$.

In particular, a mixture of pure states $d\mu_x$ and $d\mu_y, x, y \in \mathscr{M}$, is a mixed state with

$$d\mu = \alpha d\mu_x + (1 - \alpha) d\mu_y, \quad 0 < \alpha < 1$$

[20] There should be no confusion in denoting the state and the measure by μ.

so that $\sigma_\mu^2(f) > 0$ for every observable f such that $f(x) \neq f(y)$.

For a system consisting of few interacting particles (say, a motion of planets in celestial mechanics) it is possible to measure all coordinates and momenta, so one considers only pure states. Mixed states necessarily appear for macroscopic systems, when it is impossible to measure all coordinates and momenta [22].

Remark. As a topological space, the space of states $\mathscr{M}$ can be reconstructed from the algebra $\mathcal{A}$ of classical observables. Namely, suppose for simplicity that $\mathscr{M}$ is compact. Then the $\mathbb{C}$-algebra $\mathcal{C} = C(\mathscr{M})$ of complex-valued continuous functions on $\mathscr{M}$ - the completion of the complexification of the $\mathbb{R}$-algebra $\mathcal{A}$ of classical observables with respect to the sup-norm is a commutative $\mathbb{C}^*$-algebra. This means that $C(\mathscr{M})$ is a Banach space with respect to the norm $\|f\| = \sup_{x\in\mathscr{M}} |f(x)|$, has a $\mathbb{C}$-algebra structure (associative algebra over $\mathbb{C}$ with a unit) given by the point-wise product of functions such that $\|f \cdot g\| \leq \|f\|\|g\|$, and has a complex anti-linear antiinvolution: a map $^* : \mathcal{C} \to \mathcal{C}$ given by the complex conjugation $f^*(x) = \overline{f(x)}$ and satisfying $\|f \cdot f^*\| = \|f\|^2$. Then the Gelfand-Naimark theorem asserts that every commutative $\mathbb{C}^*$-algebra $\mathcal{C}$ is isomorphic to the algebra $C(\mathscr{M})$ of continuous functions on its spectrum - the set of maximal ideals of $\mathcal{C}$ - a compact topological space with the topology induced by the weak topology on $\mathcal{C}^*$, the dual space of $\mathcal{C}$.

We conclude our exposition of classical mechanics by presenting two equivalent ways of describing the dynamics - the time evolution of a Hamiltonian system $((\mathscr{M}, \{\}), H,)withthealgebraofobservables\mathcal{A} = C^\infty(\mathscr{M})$ and the set of states $\mathcal{S} = \mathscr{P}(\mathscr{M})$. In addition, we assume that the Hamiltonian phase flow g_t exists for all times, and that the phase space $\mathscr{M}$ carries a volume form dx invariant under the phase flow [23].

Hamilton's Description of Dynamics. States do not depend on time, and time evolution of observables is given by Hamilton's equations of motion,

$$\frac{d\mu}{dt} = 0, \quad \mu \in \mathcal{S}, \quad \text{and} \quad \frac{df}{dt} = \{H, f\}, \quad f \in \mathcal{A}$$

The expectation value of an observable f in the state μ at time t is given by

$$\mathrm{E}_\mu(f_t) = \int_{\mathscr{M}} f \circ g_t d\mu = \int_{\mathscr{M}} f(g_t(x))\,\rho(x)dx$$

where $\rho(x) = \frac{d\mu}{dx}$ is the Radon-Nikodim derivative. In particular, the expectation value of f in the pure state $d\mu_x$ corresponding to the point $x \in \mathscr{M}$ is $f(g_t(x))$. Hamilton's picture is commonly used for mechanical systems consisting of few interacting particles.

Liouville's Description of Dynamics. The observables do not depend on time

$$\frac{df}{dt} = 0, \quad f \in \mathcal{A},$$

and states $d\mu(x) = \rho(x)dx$ satisfy Liouville's equation

$$\frac{d\rho}{dt} = -\{H, \rho\}, \quad \rho(x)dx \in \mathcal{S}.$$

Here the Radon-Nikodim derivative $\rho(x) = \frac{d\mu}{dx}$ and Liouville's equation are understood in the distributional sense. The expectation value of an observable f in the state μ at time t is given by

[021] The space of pure states, to be precise.

[022] Typically, a macroscopic system consists of $N \sim 10^{23}$ molecules. Macroscopic systems are studied in classical statistical mechanics.

[23] It is Liouville's volume form when the Poisson structure on $\mathscr{M}$ is non-degenerate.

$$\mathrm{E}_{\mu_t}(f) = \int_{\mathscr{M}} f(x)\rho\left(g_{-t}(x)\right) dx$$

Liouville's picture, where states are described by the distribution functions $\rho(x)$ - positive distributions on $\mathscr{M}$ corresponding to probability measures $\rho(x)dx$ - is commonly used in statistical mechanics. The equality

$$\mathrm{E}_{\mu}\left(f_t\right) = \mathrm{E}_{\mu_t}(f) \quad \text{for all} \quad f \in \mathcal{A}, \quad \mu \in \mathcal{S}$$

which follows from the invariance of the volume form dx and the change of variables, expresses the equivalence between Liouville's and Hamilton's descriptions of the dynamics.

2.12.4 Connection of Classical and Quantum Mechanics

Обсудим подробно связь квантовой механики с классической.

появление принципа наименьшего действия из функционала достоверности

(below, there is a not professional attempt to explain this connection. It is still telling us something, but I don't think, that it is a fundamental one. Also, it is useless. But this is the default answer on this question from MIPT. I also don't like, how it is written, but I don't have now a better theory)

В механике частица представляет собой точку, которая движется в пространстве под воздействием сил.

В качестве наблюдаемой величины измеряется положение частицы в пространстве, которое задаётся координатой x, а зависимость от времени - траекторией $x(t)$. Лвижение полностью детерминировано, если заданы координата и скорость частицы в начальный момент времени, а также силы во всех точках пространства на протяжении всего времени их действия.

Этот факт, известный также, как принцип детерминированности в классической механике, конечно же, нашёл своё отражение в уравнениях движения частицы.

Так например, всем известное уравнение Ньютона

$$m\ddot{x} = F(t, x, \dot{x})$$

является дифференциальным уравнением второго порядка, а значит, для постановки задачи Коши для него необходимо задать начальную координату $x\left(t_0\right) = x_0$ и начальную скорость $\dot{x}\left(t_0\right) = \dot{x}_0$. Подобное описание движения частицы под действием сил представляет собой механическую формулировку принципа причинности: всякая точка на траектории частицы возникает как следствие воздействия на частицу сил в предыдущие моменты времени при заданных начальных условиях: координате и скорости в исходный момент времени.

Здесь возникает сразу несколько вопросов.

Во-первых, с чего мы взяли, что движение частицы полностью детерминировано, если в качестве начальных условий заданы только начальные координата и скорость частицы?

На самом деле, это предположение, являющееся обобщением опытных фактов, нетривиально и лежит в основе классической механики.

Во-вторых, откуда вообще взялось уравнение Ньютона и есть ли регулярный способ получения уравнений движения для механических систем?

Конечно, можно было бы просто объявить уравнение движения в форме Ньютона опытным фактом, однако, как мы увидим дальше, уравнения движения для частиц и

полей могут быть получены из такого фундаментального принципа как вариационный принцип экстремального действия Гамильтона.

Следствием этого принципа будет уравнение Эйлера- Лагранжа, которое имеет вид

$$\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = 0$$

Очевидно, что уравнение Эйлера-Лагранжа в этом случае эквивалентно уравнению Ньютона.

Действительно,

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = m\ddot{x}, \quad \frac{\partial L}{\partial x} = -\frac{\partial U}{\partial x} = F(t,x)$$

В-третьих, мы рассматриваем координаты и скорости частицы как непрерывные вещественные величины, которые в топологическом смысле определяются как множество точек с малыми окрестностями, покрывающщми область непрерывности.

Каков физический смысл этих окрестностей? Ответ на этот вопрос одновременно и прост, и сложен.

Простота в том, что в физическом смысле эти окрестности отвечают, очевидно, погрешностям измерения непрерывной величины.

В идеале окрестность может считаться бесконечно малой, но ненулевой.

Именно наличием погрешности непрерывные величины существенно отличаются от дискретных изолированных величин.

Если начальные условия для координаты и скорости частицы принимают центральные значения с конечной погрешностью, то траектории из такой малой области начальных условий могут на мальх интервалах времени либо мало отличаться от центральной траектории, либо быстро расходиться.

В последнем случае говорят, что механическая система находится в состоянии динамической неустойчивости или хаоса.

Мы ограничимся рассмотрением систем без хаоса.

Вышеупомянутая сложность в ответе на вопрос о физическом смысле окрестностей состоит в том, что неопределённость траектории может быть связана не только с инструментальной погрешностью приборов измерения наблюдаемых величин; она может иметь и казуальный характер.

Само наличие возможности задания начальных условий с инструментальной погрешностью приборов, базируется на предположении классической механики о том, что предел бесконечно малой инструментальной погрешности во всех механических системах достижим и начальные условия могут задаваться с бесконечно малой неопределённостью.

Последнее может оказаться (и оказалось в действительности при изучении этого предела в физике атомов), вообше говоря, неверным. Действительно, поставим задачу не о единичной траектории частицы, однократно зарегистрированной в измерительном приборе, а о многократных измерениях, проводимbIX одинаковыми приборами для частиц с определёнными характеристиками.

Если приборная погрешность связана с регистрацией траектории частицы, то многократная регистрация траекторий вноси’т в задачу новые характеристики.

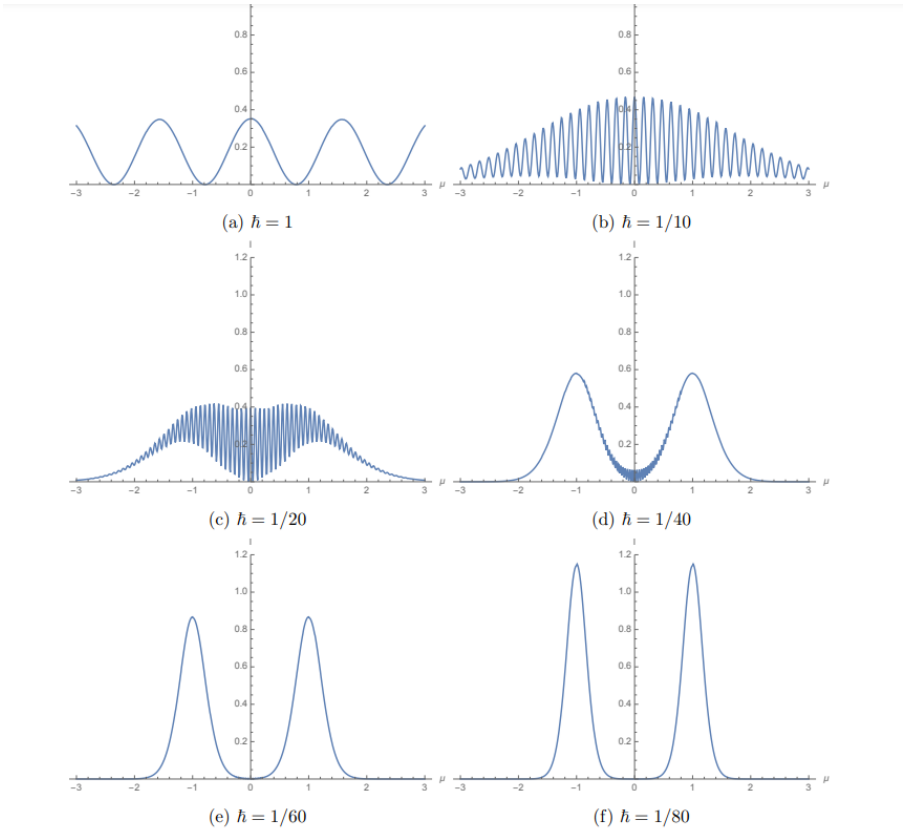
Так, например, в случае, когда свободная частица движется с некоторой скоростью равномерно и поступательно, то есть никак не взаимодействует с приборами, положение центра системы координат в приборе для свободной частицы никак не выделено и, стало быть, является неопредёленным, оно с точки зрения взаимодействия частицы с прибором абсолIотно произвольно: если в момент регистрации частицы прибором [1] поставить в приборе реперну ю точку, которая будет измерена с инструментальной

погрешностью самого прибора, то многократные повторы регистрации дадут некую форму распределения вероятности расположения реперных точек в приборе. ’ ’то распределение будет иметь свои погрешности и другие вероятностные характеристики многократных измерений в зависимости от физики источника свободной частицы.

Other questions about connection of classical and quantum mechanics

О переходе в классику популярно (!??!?!??!??!)

(напишу, типичный вопрос)



(a) $\hbar = 1$ (b) $\hbar = 1/10$ (c) $\hbar = 1/20$ (d) $\hbar = 1/40$ (e) $\hbar = 1/60$ (f) $\hbar = 1/80$

3 Formalism of Quantum Mechanics

3.1 Basic Principles of Quantum Mechanics

3.1.1 Observables, States, and Dynamics

Quantum mechanics studies the microworld - the physical laws at an atomic scale - that cannot be adequately described by classical mechanics. The properties of the microworld are so different from our everyday experiences that it is no surprise that its laws seem to contradict the common sense. Thus classical mechanics and classical electrodynamics cannot explain the stability of atoms and molecules. Neither can these theories reconcile different properties of light, its wave-like behavior in interference and diffraction phenomena, and its particle-like behavior in photo-electric emission and scattering by free photons. The fundamental difference between the microworld and the perceived world around us is that in the microworld every experiment results in interaction with the system and thus disturbs its properties, whereas in classical physics it is always assumed that one can neglect the disturbances the measurement

brings upon a system. This imposes a limitation on our powers of observation and leads to a conclusion that there exist observables which cannot be measured simultaneously.

We will not discuss here these and other basic experimental facts, referring the interested reader to physics textbooks. Nor will we follow the historic path of the theory. Instead, we show how to formulate quantum mechanics using the general notions of states, observables, and time evolution, described in Section 2.8 in Chapter 1. There we have seen that commutativity of the algebra of observables $\mathcal{A}$ results in its realization as an algebra of functions on the topological space - the space of states - and thus brings us to the realm of classical mechanics. Therefore in order to get a realization of observables and states which is different from classical mechanics, we must assume that the $\mathbb{C}^*$-algebra associated with observables is no longer commutative. A fundamental example of a non-commutative $\mathbb{C}^*$-algebra is given by the algebra of all bounded operators on a complex Hilbert space, and it turns out that it is this algebra which plays a fundamental role in quantum mechanics!

Here we formulate the basic principles of quantum mechanics using precise mathematical language. At this point it should be noted that one can not verify directly the principles lying at the foundation of quantum mechanics. Nevertheless, the validity of quantum mechanics, whenever it is applicable, is continuously being confirmed by numerous experimental facts which perfectly agree with the predictions of the theory [7].

1.1. Mathematical formulation.

The following axioms constitute the basis of quantum mechanics.

A1. With every quantum system there is associated an infinite-dimensional separable complex Hilbert space $\mathscr{H}$, in physics terminology called the space of states [8]. The Hilbert space of a composite quantum system is a tensor product of Hilbert spaces of component systems.

A2. The set of observables $\mathscr{A}$ of a quantum system with the Hilbert space $\mathscr{H}$ consists of all self-adjoint operators on $\mathscr{H}$. The subset $\mathscr{A}_0 = \mathscr{A} \cap \mathscr{L}(\mathscr{H})$ of bounded observables is a vector space over $\mathbb{R}$.

A3. The set of states $\mathscr{S}$ of a quantum system with a Hilbert space $\mathscr{H}$ consists of all positive (and hence self-adjoint) trace class operators M with

$\operatorname{Tr} M = 1$. Pure states are projection operators onto one-dimensional subspaces of $\mathscr{H}$. For $\psi \in \mathscr{H}, \|\psi\| = 1$, the corresponding projection onto $\mathbb{C}\psi$ is denoted by P_ψ. All other states are called mixed states [9].

A4. A process of measurement is the correspondence

$$\mathscr{A} \times \mathscr{S} \ni (A, M) \mapsto \mu_A \in \mathscr{P}(\mathbb{R})$$

which to every observable $A \in \mathscr{A}$ and state $M \in \mathscr{S}$ assigns a probability measure μ_A on $\mathbb{R}$. For every Borel subset $E \subseteq \mathbb{R}$, the quantity $0 \leq \mu_A(E) \leq 1$ is the probability that for a quantum system in the state M the result of a measurement of the observable A belongs to E. The expectation value (the mean-value) of the observable $A \in \mathscr{A}$ in the state $M \in \mathscr{S}$ is

$$\langle A|M\rangle = \int_{-\infty}^{\infty} \lambda d\mu_A(\lambda)$$

where $\mu_A(\lambda) = \mu_A((-\infty, \lambda))$ is a distribution function for the probability measure μ_A.

The set of states $\mathscr{S}$ is a convex set. According to the Hilbert-Schmidt theorem on the canonical decomposition for compact self-adjoint operators, for every $M \in \mathscr{S}$ there exists an orthonormal set $\{\psi_n\}_{n=1}^N$ in $\mathscr{H}$ (finite or infinite, in the latter case $N = \infty$) such that

[07] This refers to non-relativistic phenomena at the atomic scale.

[8] The space of pure states, to be precise.

$$M = \sum_{n=1}^{N} \alpha_n P_{\psi_n} \quad \text{and} \quad \operatorname{Tr} M = \sum_{n=1}^{N} \alpha_n = 1 \tag{1.1}$$

where $\alpha_n > 0$ are non-zero eigenvalues of M. Thus every mixed state is a convex linear combination of pure states. The following result characterizes the pure states.

Lemma 1.1. A state $M \in \mathscr{S}$ is a pure state if and only if it cannot be represented as a non-trivial convex linear combination in $\mathscr{S}$.

Proof. Suppose that

$$P_\psi = aM_1 + (1-a)M_2, \quad 0 < a < 1,$$

and let $\mathscr{H} = \mathbb{C}\psi \oplus \mathscr{H}_1$ be the orthogonal sum decomposition. Since M_1 and M_2 are positive operators, for $\varphi \in \mathscr{H}_1$ we have

$$a\,(M_1\varphi, \varphi) \le (P_\psi \varphi, \varphi) = 0$$

so that $(M_1\varphi, \varphi) = 0$ for all $\varphi \in \mathscr{H}_1$ and by (0.1) we get $M_1|_{\mathscr{H}_1} = 0$. Since M_1 is self-adjoint, it leaves the complementary subspace $\mathbb{C}\psi$ invariant, and from $\operatorname{Tr} M_1 = 1$ it follows that $M_1 = P_\psi$. Therefore, $M_1 = M_2 = P_\psi$.

Explicit construction of the correspondence $\mathscr{A} \times \mathscr{S} \to \mathscr{P}(\mathbb{R})$ is based on the general spectral theorem of von Neumann, which emphasizes the fundamental role the self-adjoint operators play in quantum mechanics.

Definition. A projection-valued measure on $\mathbb{R}$ is a mapping $\mathrm{P} : \mathscr{B}(\mathbb{R}) \to \mathscr{L}(\mathscr{H})$ of the σ-algebra $\mathscr{B}(\mathbb{R})$ of Borel subsets of $\mathbb{R}$ into the algebra of bounded operators on $\mathscr{H}$, satisfying the following properties.

PM1. For every Borel subset $E \subseteq \mathbb{R}, \mathrm{P}(E)$ is an orthogonal projection, i.e., $\mathrm{P}(E) = \mathrm{P}(E)^2$ and $\mathrm{P}(E) = \mathrm{P}(E)^*$.

PM2. $\mathrm{P}(\emptyset) = 0, \mathrm{P}(\mathbb{R}) = I$, the identity operator on $\mathscr{H}$.

PM3. For every disjoint union of Borel subsets,

$$E = \coprod_{n=1}^{\infty} E_n, \quad \mathrm{P}(E) = \lim_{n\to\infty} \sum_{i=1}^{n} \mathrm{P}\,(E_i)$$

in the strong topology on $\mathscr{L}(\mathscr{H})$.

Remark. Similarly, a projection-valued measure on $\mathbb{R}^n$ is a mapping P: $\mathscr{B}\,(\mathbb{R}^n) \to \mathscr{L}(\mathscr{H})$, satisfying the same properties PM1-PM3.

It follows from PM1-PM3 that

$$\mathrm{P}\,(E_1)\,\mathrm{P}\,(E_2) = \mathrm{P}\,(E_1 \cap E_2) \quad \text{for all } E_1, E_2 \in \mathscr{B}(\mathbb{R}) \tag{1.2}$$

With every projection-valued measure P on $\mathbb{R}$ we associate a projectionvalued function

$$\mathrm{P}(\lambda) = \mathrm{P}((-\infty, \lambda)),$$

called the projection-valued resolution of the identity. It is characterized by the following properties.

PD1.

$$\mathrm{P}(\lambda)\mathrm{P}(\mu) = \mathrm{P}(\min\{\lambda, \mu\})$$

[09] In physics terminology, the operator M is called the density operator.

PD2.

$$\lim_{\lambda\to-\infty} \mathrm{P}(\lambda) = 0, \quad \lim_{\lambda\to\infty} \mathrm{P}(\lambda) = I$$

PD3.

$$\lim_{\substack{\mu\to\lambda \\ \mu<\lambda}} \mathrm{P}(\mu) = \mathrm{P}(\lambda).$$

For every $\varphi \in \mathscr{H}$ the resolution of the identity $\mathrm{P}(\lambda)$ defines a distribution function $(\mathrm{P}(\lambda)\varphi, \varphi)$ of the bounded measure on $\mathbb{R}$ (probability measure when $\|\varphi\| = 1$). By the polarization identity

$$\begin{aligned}(\mathrm{P}(\lambda)\varphi, \psi) = \frac{1}{4}\{&(\mathrm{P}(\lambda)(\varphi+\psi), \varphi+\psi) - (\mathrm{P}(\lambda)(\varphi-\psi), \varphi-\psi) \\ &+ i(\mathrm{P}(\lambda)(\varphi+i\psi), \varphi+i\psi) - i(\mathrm{P}(\lambda)(\varphi-i\psi), \varphi-i\psi)\}\end{aligned}$$

so that $(\mathrm{P}(\lambda)\varphi, \psi)$ corresponds to a complex measure on $\mathbb{R}$ - a complex linear combination of measures.

A measurable function f on $\mathbb{R}$ is said to be finite almost everywhere (a.e.) with respect to the projection-valued measure P if it is finite a.e. with respect to all measures $(\mathrm{P}\psi, \psi), \psi \in \mathscr{H}$. For separable $\mathscr{H}$ a theorem of von Neumann states that for every projection-valued measure P there exists $\varphi \in \mathscr{H}$ such that a function f is finite a.e. with respect to P if and only if it is finite a.e. with respect to the measure $(\mathrm{P}\varphi, \varphi)$.

The next statement is the celebrated general spectral theorem of von Neumann.

Theorem 1.1 (J. von Neumann). For every self-adjoint operator A on the Hilbert space $\mathscr{H}$ there exists a unique projection-valued resolution of the identity $\mathrm{P}(\lambda)$, satisfying the following properties.
(i)

$$D(A) = \left\{\varphi \in \mathscr{H} : \int_{-\infty}^{\infty} \lambda^2 d(\mathrm{P}(\lambda)\varphi, \varphi) < \infty\right\},$$

and for every $\varphi \in D(A)$

$$A\varphi = \int_{-\infty}^{\infty} \lambda d\mathrm{P}(\lambda)\varphi,$$

defined as a limit of Riemann-Stieltjes sums in the strong topology on $\mathscr{H}$. The support of the corresponding projection-valued measure P coincides with the spectrum of the operator $A : \lambda \in \sigma(A)$ if and only if $\mathrm{P}_A((\lambda-\varepsilon, \lambda+\varepsilon)) \neq 0$ for all $\varepsilon > 0$.
(ii) For every continuous function f on $\mathbb{R}$, $f(A)$ is a linear operator on $\mathscr{H}$ with a dense domain

$$D(f(A)) = \left\{\varphi \in \mathscr{H} : \int_{-\infty}^{\infty} |f(\lambda)|^2 d(\mathrm{P}(\lambda)\varphi, \varphi) < \infty\right\}$$

defined for $\varphi \in D(f(A))$ as

$$f(A)\varphi = \int_{-\infty}^{\infty} f(\lambda) d\mathrm{P}(\lambda)\varphi,$$

and understood as in part (i). The operator $f(A)$ satisfies

$$f(A)^* = \bar{f}(A)$$

where $\bar{f}$ is the complex conjugate function to f, and the operator $f(A)$ is bounded if and only if the function f is bounded on $\sigma(A)$. For bounded on $\sigma(A)$ continuous functions f and g,

$$f(A)g(A)\varphi = \int_{-\infty}^{\infty} f(\lambda)g(\lambda)d\mathrm{P}(\lambda)\varphi, \quad \varphi \in \mathscr{H}.$$

(iii) For every measurable function f on $\mathbb{R}$, finite a.e. with respect to the projection-valued measure P, $f(A)$ is a linear operator on $\mathscr{H}$ defined as in (ii), where the integral for $f(A)\varphi$ is now understood in the weak sense: for $\varphi \in D(f(A))$ and every $\psi \in \mathscr{H}$,

$$(f(A)\varphi, \psi) = \int_{-\infty}^{\infty} f(\lambda)d(\mathrm{P}(\lambda)\varphi, \psi)$$

- a Lebesgue-Stieltjes integral with respect to a complex measure. The correspondence $f \mapsto f(A)$ satisfies the same properties as in (ii), where the integrals are understood in the weak sense.
  (iv) A bounded operator B commutes with A, that is, $B(D(A)) \subset D(A)$ and $AB = BA$ on $D(A)$, if and only if it commutes with $\mathrm{P}(\lambda)$ for all λ and, therefore, B commutes with every operator $f(A)$.
  (v) For every projection-valued resolution of identity $\mathrm{P}(\lambda)$ the operator A on $\mathscr{H}$, defined as in part (i), is self-adjoint.

Using the spectral theorem, the correspondence $(A, M) \mapsto \mu_A$, postulated in A4, can be explicitly described as follows.

A5. The probability measure μ_A on $\mathbb{R}$, which defines the correspondence $\mathscr{A} \times \mathscr{S} \to \mathscr{P}(\mathbb{R})$, is given by the Born-von Neumann formula

$$\mu_A(E) = \operatorname{Tr} P_A(E)M, \quad E \in \mathscr{B}(\mathbb{R}) \tag{1.3}$$

where P_A is a projection-valued measure on $\mathbb{R}$ associated with the self-adjoint operator A.

Remark. The probability measure μ_A on $\mathbb{R}$ can be considered as a "quantum push-forward" of the state M by the observable A (cf. the discussion in Section 2.8 in Chapter 1).

From the Hilbert-Schmidt decomposition (1.1) we get

$$\mu_A(E) = \sum_{n=1}^{N} \alpha_n \left(\mathrm{P}_A(E)\psi_n, \psi_n\right) = \sum_{n=1}^{N} \alpha_n \left\|\mathrm{P}_A(E)\psi_n\right\|^2 \leq \sum_{n=1}^{N} \alpha_n = 1$$

so that indeed $0 \leq \mu_A(E) \leq 1$. Denote by $\mu_A(\lambda)$ the distribution function of the probability measure μ_A, $\mu_A(\lambda) = (\mathrm{P}_A(\lambda)\psi, \psi)$ for $M = P_\psi$.

Proposition 1.1. Suppose that an observable $A \in \mathscr{A}$ and a state $M \in \mathscr{S}$ are such that $\langle A|M\rangle < \infty$ and $\operatorname{Im} M \subseteq D(A)$. Then $AM \in \mathscr{S}_1$ and

$$\langle A|M\rangle = \operatorname{Tr} AM$$

In particular, if $M = P_\psi$ and $\psi \in D(A)$, then

$$\langle A|M\rangle = (A\psi, \psi) \quad \text{and} \quad \left\langle A^2|M\right\rangle = \|A\psi\|^2.$$

Proof. Let $\{e_n\}_{n=1}^{\infty}$ be an orthonormal basis for $\mathscr{H}$. Since

$$\mu_A(E) = \operatorname{Tr} \mathrm{P}_A(E)M = \sum_{n=1}^{\infty} \left(\mathrm{P}_A(E)Me_n, e_n\right)$$

we get for every $E \in \mathscr{B}(\mathbb{R})$,

$$\mu_A(E) = \sum_{n=1}^{\infty} \mu_n(E)$$

where μ_n are finite measures on $\mathbb{R}$ defined by $\mu_n(E) = (\mathrm{P}_A(E)Me_n, e_n)$. Since

$$\int_{\mathbb{R}} f d\mu_A = \sum_{n=1}^{\infty} \int_{\mathbb{R}} f d\mu_n$$

for every function f integrable with respect to the measure μ_A, it follows from the spectral theorem that

$$\sum_{n=1}^{\infty} (AMe_n, e_n) = \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \lambda d\mu_n(\lambda) = \int_{-\infty}^{\infty} \lambda d\mu_A(\lambda) < \infty$$

Thus $AM \in \mathscr{S}_1$ and $\langle A|M\rangle = \operatorname{Tr} AM$. In particular, when $M = P_\psi$ and $\psi \in D(A)$,

$$\langle A|M\rangle = \int_{-\infty}^{\infty} \lambda d\left(\mathrm{P}_A(\lambda)\psi, \psi\right) = (A\psi, \psi)$$

Finally, from the spectral theorem and the change of variables formula we get

$$\|A\psi\|^2 = \int_{-\infty}^{\infty} \lambda^2 d\left(\mathrm{P}_A(\lambda)\psi, \psi\right) = \int_0^{\infty} \lambda d\left(\mathrm{P}_{A^2}(\lambda)\psi, \psi\right) = \left\langle A^2|M\right\rangle$$

Corollary 1.2. If $\langle A|M\rangle, \langle A^2|M\rangle < \infty$, then $AM \in \mathscr{S}_1$ and $\langle A|M\rangle = \operatorname{Tr} AM$.

Proof. Since

$$\int_{-\infty}^{\infty} \lambda^2 d\mu_n(\lambda) \le \int_{-\infty}^{\infty} \lambda^2 d\mu_A(\lambda) = \left\langle A^2|M\right\rangle < \infty$$

we get that $e_n \in D(AM)$, and the result follows from the proof of Proposition 1.1.

Remark. It is convenient to approximate an unbounded self-adjoint operator A by bounded operators $A_n = f_n(A)$, where $f_n = \chi_{[-n,n]}$ - a characteristic function of the interval $[-n, n]$. Assuming that $\langle A|M\rangle$ exists, we have

$$\langle A|M\rangle = \int_{-\infty}^{\infty} \lambda d\mu_A(\lambda) = \lim_{n\to\infty} \int_{-n}^{n} \lambda d\mu_A(\lambda) = \lim_{n\to\infty} \langle A_n|M\rangle$$

Definition. Self-adjoint operators A and B commute if the corresponding projection-valued measures P_A and P_B commute,

$$\mathrm{P}_A(E_1)\,\mathrm{P}_B(E_2) = \mathrm{P}_B(E_2)\,\mathrm{P}_A(E_1) \quad \text{for all} \quad E_1, E_2 \in \mathscr{B}(\mathbb{R})$$

The following results, which follow from the spectral theorem, are very useful in applications.

Proposition 1.2. The following statements are equivalent.

(i) Self-adjoint operators A and B commute.

(ii) For all $\lambda, \mu \in \mathbb{C}, \operatorname{Im}\lambda, \operatorname{Im}\mu \neq 0$,

$$R_\lambda(A)R_\mu(B) = R_\mu(B)R_\lambda(A)$$

(iii) For all $u, v \in \mathbb{R}$,

$$e^{iuA}e^{ivB} = e^{ivB}e^{iuA}.$$

(iv) For all $u \in \mathbb{R}$, the operators e^{iuA} and B commute.

Slightly abusing notation [10], we will often write $[A, B] = AB - BA = 0$ for commuting self-adjoint operators A and B.

Proposition 1.3. Let $\boldsymbol{A} = \{A_1, ..., A_n\}$ be a finite set of self-adjoint, pairwise commuting operators on $\mathscr{H}$. There exists a unique projection-valued measure $\mathrm{P}_{\boldsymbol{A}}$ on the Borel subsets of $\mathbb{R}^n$ having the following properties.
(i) For every $\boldsymbol{E} = E_1 \times \cdots \times E_n \in \mathscr{B}(\mathbb{R}^n)$,

$$\mathrm{P}_{\boldsymbol{A}}(\boldsymbol{E}) = \mathrm{P}_{A_1}(E_1) ... \mathrm{P}_{A_n}(E_n).$$

(ii) In the strong operator topology,

$$A_k = \int_{\mathbb{R}^n} \lambda_k d\mathrm{P}_{\boldsymbol{A}}, \quad k = 1, ..., n$$

where λ_k is the k-th coordinate function on $\mathbb{R}^n$, $\lambda_k(x_1, ..., x_n) = x_k$.
(iii) For every measurable function f on $\mathbb{R}^n$, finite a.e. with respect to the projection-valued measure $\mathrm{P}_{\boldsymbol{A}}$, $f(A_1, ..., A_n)$ is a linear operator on $\mathscr{H}$ defined *by*

$$f(A_1, ..., A_n) = \int_{\mathbb{R}^n} f d\mathrm{P}_{\boldsymbol{A}}$$

where the integral is understood in the weak operator topology. The correspondence $f \mapsto f(A_1, ..., A_n)$ satisfies the same properties as in part (ii) of the spectral theorem.

The support of the projection-valued measure $\mathrm{P}_{\boldsymbol{A}}$ on $\mathbb{R}^n$ is called the joint spectrum of the commutative family $\boldsymbol{A} = \{A_1, ..., A_n\}$.

Remark. According to von Neumann's theorem on a generating operator, for every commutative family $\boldsymbol{A}$ of self-adjoint operators (not necessarily finite) on a separable Hilbert space $\mathscr{H}$ there is a generating operator - a self-adjoint operator R on $\mathscr{H}$ such that all operators in A are functions of R.

It seems natural that simultaneous measurement of a finite set of observables $\boldsymbol{A} = \{A_1, ..., A_n\}$ in the state $M \in \mathscr{S}$ should be described by the probability measure μ_A on $\mathbb{R}^n$ given by the following generalization of the Born-von Neumann formula:
(1.4) $\mu_{\boldsymbol{A}}(\boldsymbol{E}) = \mathrm{Tr}\left(\mathrm{P}_{A_1}(E_1) ... \mathrm{P}_{A_n}(E_n) M\right), \quad \boldsymbol{E} = E_1 \times \cdots \times E_n \in \mathscr{B}(\mathbb{R}^n)$.

However, formula (1.4) defines a probability measure on $\mathbb{R}^n$ if and only if $\mathrm{P}_{A_1}(E_1) ... \mathrm{P}_{A_n}(E_n)$ defines a projection-valued measure on $\mathbb{R}^n$. Since a product of orthogonal projections is an orthogonal projection only when the projection operators commute, we conclude that the operators $A_1, ..., A_n$ should form a commutative family. This agrees with the requirement that simultaneous measurement of several observables should be independent of the order of the measurements of individual observables. We summarize these arguments as the following axiom.

A6. A finite set of observables $\boldsymbol{A} = \{A_1, ..., A_n\}$ can be measured simultaneously (simultaneously measured observables) if and only if they form a commutative family. Simultaneous measurement of the commutative family $\boldsymbol{A} \subset \mathscr{A}$ in the state $M \in \mathscr{S}$ is described by the probability measure $\mu_{\boldsymbol{A}}$ on $\mathbb{R}^n$ given by

$$\mu_{\boldsymbol{A}}(\boldsymbol{E}) = \mathrm{Tr}\, \mathrm{P}_{\boldsymbol{A}}(\boldsymbol{E}) M, \quad \boldsymbol{E} \in \mathscr{B}(\mathbb{R}^n),$$

where P_A is the projection-valued measure from Proposition 1.3. Explicitly, $\mathrm{P}_{\boldsymbol{A}}(\boldsymbol{E}) = \mathrm{P}_{A_1}(E_1) ... \mathrm{P}_{A_n}(E_n)$ for $\boldsymbol{E} = E_1 \times \cdots \times E_n \in \mathscr{B}(\mathbb{R}^n)$. For every Borel subset $\boldsymbol{E} \subseteq \mathbb{R}^n$ the

[010] In general, for unbounded self-adjoint operators A and B the commutator $[A, B] - AB - BA$ is not necessarily closed, i.e., it could be defined only for $\varphi = 0$.

quantity $0 \le \mu_{\boldsymbol{A}}(\boldsymbol{E}) \le 1$ is the probability that for a quantum system in the state M the result of the simultaneous measurement of observables $A_1, ..., A_n$ belongs to $\boldsymbol{E}$.

The axioms A1-A6 are known as Dirac-von Neumann axioms.

Problem 1.1. Prove property (1.2).

Problem 1.2. Prove that the state M is a pure state if and only if $\operatorname{Tr} M^2 = 1$.

Problem 1.3. Prove that the Born-von Neumann formula (1.3) defines a probability measure on $\mathbb{R}$, i.e., μ_A is a σ-additive function on $\mathscr{B}(\mathbb{R})$.

Problem 1.4. Prove all the remaining statements in this section.

1.2. Heisenberg's uncertainty relations. The variance of the observable A in the state M, which measures the mean deviation of A from its expectation value, is defined by

$$\sigma_M^2(A) = \left\langle (A - \langle A|M\rangle I)^2 | M \right\rangle = \left\langle A^2 | M \right\rangle - \langle A|M\rangle^2 \ge 0$$

provided the expectation values $\langle A^2|M\rangle$ and $\langle A|M\rangle$ exist. It follows from Proposition 1.1 that for $M = P_\psi$, where $\psi \in D(A)$,

$$\sigma_M^2(A) = \|(A - \langle A|M\rangle I)\psi\|^2 = \|A\psi\|^2 - (A\psi, \psi)^2$$

Lemma 1.2. For $A \in \mathscr{A}$ and $M \in \mathscr{S}$ the variance $\sigma_M(A) = 0$ if and only if $\operatorname{Im} M$ is an eigenspace for the operator A with the eigenvalue $a = \langle A|M\rangle$. In particular, if $M = P_\psi$, then ψ is an eigenvector of A, $A\psi = a\psi$.

Proof. It follows from the spectral theorem that

$$\sigma_M^2(A) = \int_{-\infty}^{\infty} (\lambda - a)^2 d\mu_A(\lambda)$$

so that $\sigma_M(A) = 0$ if and only if the probability measure μ_A is supported at the point $a \in \mathbb{R}$, i.e., $\mu_A(\{a\}) = 1$. Since $\mu_A(\{a\}) = \operatorname{Tr} P_A(\{a\})M$ and $\operatorname{Tr} M = 1$, we conclude that this is equivalent to $\operatorname{Im} M$ being an invariant subspace for $P_A(\{a\})$, and it follows from the spectral theorem that $\operatorname{Im} M$ is an eigenspace for A with the eigenvalue a.

Generalized Heisenberg's uncertainty relations

Now we formulate generalized Heisenberg's uncertainty relations.

Proposition 1.4 (H. Weyl).

Let $A, B \in \mathscr{A}$ and let $M = P_\psi$ be the pure state such that $\psi \in D(A) \cap D(B)$ and $A\psi, B\psi \in D(A) \cap D(B)$. Then

$$\sigma_M^2(A)\sigma_M^2(B) \ge \frac{1}{4}\langle i[A, B]|M\rangle^2$$

The same inequality holds for all $M \in \mathscr{S}$, where by definition $\langle i[A, B]|M\rangle = \lim_{n\to\infty} \langle i\,[A_n, B_n]\,|M\rangle$.

Proof. Let $M = P_\psi$. Since

$$[A - \langle A|M\rangle I, B - \langle B|M\rangle I] = [A, B]$$

it is sufficient to prove the inequality

$$\left\langle A^2|M\right\rangle \left\langle B^2|M\right\rangle \ge \frac{1}{4}\langle i[A, B]|M\rangle^2.$$

We have for all $\alpha \in \mathbb{R}$,

$$\|(A+i\alpha B)\psi\|^2 = \alpha^2(B\psi,B\psi) - i\alpha(A\psi,B\psi) + i\alpha(B\psi,A\psi) + (A\psi,A\psi)$$
$$= \alpha^2\left(B^2\psi,\psi\right) + \alpha(i[A,B]\psi,\psi) + \left(A^2\psi,\psi\right) \geq 0$$

so that necessarily $4\left(A^2\psi,\psi\right)\left(B^2\psi,\psi\right) \geq (i[A,B]\psi,\psi)^2$.

The same argument works for the mixed states. Since

$$\sigma_M^2(A)\sigma_M^2(B) = \lim_{n\to\infty} \sigma_M^2\left(A_n\right)\sigma_M^2\left(B_n\right)$$

(see the remark in the previous section), it is sufficient to prove the inequality for bounded A and B. Then using the cyclic property of the trace we have for all $\alpha \in \mathbb{R}$,

$$0 \leq \operatorname{Tr}\left((A+i\alpha B)M(A+i\alpha B)^*\right) = \operatorname{Tr}((A+i\alpha B)M(A-i\alpha B))$$
$$= \alpha^2 \operatorname{Tr} BMB + i\alpha \operatorname{Tr} BMA - i\alpha \operatorname{Tr} AMB + \operatorname{Tr} AMA$$
$$= \alpha^2 \operatorname{Tr} B^2M + \alpha \operatorname{Tr}(i[A,B]M) + \operatorname{Tr} A^2M,$$

so that $4 \operatorname{Tr} A^2M \operatorname{Tr} B^2M \geq \operatorname{Tr}(i[A,B]M)^2$.

Heisenberg's uncertainty relations provide a quantitative expression of the fact that even in a pure state non-commuting observables cannot be measured simultaneously. This shows a fundamental difference between the process of measurement in classical mechanics and in quantum mechanics.

1.3. Dynamics.

The set $\mathscr{A}$ of quantum observables does not form an algebra with respect to an operator product [11]. Nevertheless, a real vector space $\mathscr{A}_0$ of bounded observables has a Lie algebra structure with the Lie bracket

$$i[A,B] = i(AB-BA), \quad A,B \in \mathscr{A}_0$$

Remark. In fact, the $\mathbb{C}^*$-algebra $\mathscr{L}(\mathscr{H})$ of bounded operators on $\mathscr{H}$ has a structure of a complex Lie algebra with the Lie bracket given by a commutator $[A,B] = AB-BA$. It satisfies the Leibniz rule

$$[AB,C] = A[B,C] + [A,C]B$$

so that the Lie bracket is a derivation of the $\mathbb{C}^*$-algebra $\mathscr{L}(\mathscr{H})$.

In analogy with classical mechanics, we postulate that the time evolution of a quantum system with the space of states $\mathscr{H}$ is completely determined by a special observable $H \in \mathscr{A}$, called a Hamiltonian operator (Hamiltonian for brevity). As in classical mechanics, the Lie algebra structure on $\mathscr{A}_0$ leads to corresponding quantum equations of motion.

Specifically, the analog of Hamilton's picture in classical mechanics (see Section 2.8 in Chapter 1) is the Heisenberg picture in quantum mechanics, where the states do not depend on time

$$\frac{dM}{dt} = 0, \quad M \in \mathscr{S}$$

and bounded observables satisfy the Heisenberg equation of motion

$$\frac{dA}{dt} = \{H,A\}_\hbar, \quad A \in \mathscr{A}_0, \tag{1.5}$$

[011] The product of two non-commuting self-adjoint operators is not self-adjoint.

where

$$\{,\}_\hbar = \frac{i}{\hbar}[,] \tag{1.6}$$

is the quantum bracket - the $\hbar$-dependent Lie bracket on $\mathscr{A}_0$. The positive number $\hbar$, called the Planck constant, is one of the fundamental constants in physics [12].

The Heisenberg equation (1.5) is well defined when $H \in \mathscr{A}_0$. Indeed, let $U(t)$ be a strongly continuous one-parameter group of unitary operators associated with a bounded self-adjoint operator H,

$$U(t) = e^{-\frac{i}{\hbar}tH}, \quad t \in \mathbb{R} \tag{1.7}$$

It satisfies the differential equation

$$i\hbar\frac{dU(t)}{dt} = HU(t) = U(t)H \tag{1.8}$$

so that the solution $A(t)$ of the Heisenberg equation of motion with the initial condition $A(0) = A \in \mathscr{A}_0$ is given by

$$A(t) = U(t)^{-1}AU(t) \tag{1.9}$$

In general, a strongly one-parameter group of unitary operators (1.7), associated with a self-adjoint operator H, satisfies differential equation (1.8) only on $D(H)$ in a strong sense, that is, applied to $\varphi \in D(H)$. The quantum dynamics is defined by the same formula (1.9), and in this sense all quantum observables satisfy the Heisenberg equation of motion (1.5). The evolution operator $U_t : \mathscr{A} \to \mathscr{A}$ is defined by $U_t(A) = A(t) = U(t)^{-1}AU(t)$, and is an automorphism of the Lie algebra $\mathscr{A}_0$ of bounded observables. This is a quantum analog of the statement that the evolution operator in classical mechanics is an automorphism of the Poisson algebra of classical observables (see Theorem 2.19 in Section 2.7 of Chapter 1).

By Stone's theorem, every strongly-continuous one-parameter group of unitary operators [13]$U(t)$ is of the form (1.7), where
$D(H) = \left\{\varphi \in \mathscr{H} : \lim_{t\to 0}\frac{U(t)-I}{t}\varphi \text{ exists } \right\}$ and $H\varphi = i\hbar\lim_{t\to 0}\frac{U(t)-I}{t}\varphi$.
The domain $D(H)$ of the self-adjoint operator H, called the infinitesimal generator of $U(t)$, is an invariant linear subspace for all operators $U(t)$.

We summarize the presented arguments as the following axiom.

A7 (Heisenberg's Picture). The dynamics of a quantum system is described by the strongly continuous one-parameter group $U(t)$ of unitary operators. Quantum states do not depend on time, $\mathscr{S} \ni M \mapsto M(t) = M \in \mathscr{S}$, and time dependence of quantum observables is given by the evolution operator U_t,

$$\mathscr{A} \ni A \mapsto A(t) = U_t(A) = U(t)^{-1}AU(t) \in \mathscr{A}.$$

Infinitesimally, the evolution of quantum observables is described by the Heisenberg equation of motion (1.5), where the Hamiltonian operator H is the infinitesimal generator of $U(t)$.

The analog of Liouville's picture in classical mechanics (see Section 2.8 in Chapter 1) is Schrodinger's picture in quantum mechanics, defined as follows.

[012] The Planck constant has a physical dimension of the action (energy $\times$ time). Its value $\hbar = 1.054 \times 10^{-27}$erg $\times$ sec, which is determined from the experiment, manifests that quantum mechanics is a microscopic theory.

[13] According to a theorem of von Neumann, on a separable Hilbert space every weakly measurable one-parameter group of unitary operators is strongly continuous.

A8 (Schrodinger's Picture). The dynamics of a quantum system is described by the strongly continuous one-parameter group $U(t)$ of unitary operators. Quantum observables do not depend on time, $\mathscr{A} \ni A \mapsto A(t) = A \in \mathscr{A}$, and time dependence of states is given by the inverse of the evolution operator $U_t^{-1} = U_{-t}$,

$$\mathscr{S} \ni M \mapsto M(t) = U_{-t}(M) = U(t)MU(t)^{-1} \in \mathscr{S}. \tag{1.10}$$

Infinitesimally, the evolution of quantum states is described by the Schrodinger equation of motion

$$\frac{dM}{dt} = -\{H, M\}_h, \quad M \in \mathscr{S} \tag{1.11}$$

where the Hamiltonian operator H is the infinitesimal generator of $U(t)$.

Proposition 1.5. Heisenberg and Schrodinger descriptions of dynamics are equivalent.

Proof. Let $\mu_{A(t)}$ and $(\mu_t)_A$ be, respectively, probability measures on $\mathbb{R}$ associated with $(A(t), M) \in \mathscr{A} \times \mathscr{S}$ and $(A, M(t)) \in \mathscr{A} \times \mathscr{S}$ according to A3-A4, where $A(t) = U_t(A)$ and $M(t) = U_{-t}(M)$. We need to show that $\mu_{A(t)} = (\mu_t)_A$. It follows from the spectral theorem that $\mathrm{P}_{A(t)} = U(t)^{-1}\mathrm{P}_A U(t)$, so that using the Born-von Neumann formula (1.3) and the cyclic property of the trace, we get for $E \in \mathscr{B}(\mathbb{R})$,

$$\begin{aligned}\mu_{A(t)}(E) &= \operatorname{Tr} \mathrm{P}_{A(t)}(E)M = \operatorname{Tr}\left(U(t)^{-1}\mathrm{P}_A(E)U(t)M\right) \\ &= \operatorname{Tr}\left(\mathrm{P}_A(E)U(t)MU(t)^{-1}\right) = \operatorname{Tr}\mathrm{P}_A(E)M(t) = (\mu_t)_A(E)\end{aligned}$$

Corollary 1.3. $\langle A(t)|M\rangle = \langle A|M(t)\rangle$.

In analogy with classical mechanics (see Section 1.4 of Chapter 1), we have the following definition.

Definition. An observable $A \in \mathscr{A}$ is a quantum integral of motion (or a constant of motion) for a quantum system with the Hamiltonian H if in Heisenberg's picture

$$\frac{dA(t)}{dt} = 0$$

It follows from Proposition 1.2 that $A \in \mathscr{A}$ is an integral of motion if and only if it commutes with the Hamiltonian H, so that, in agreement with (1.5),

$$\{H, A\}_\hbar = 0$$

This is a quantum analog of the Poisson commutativity property, given by formula (2.14) in Section 2.6 of Chapter 1.

It follows from (1.11) that the time evolution of a pure state $M = P_\psi$ is given by $M(t) = P_{\psi(t)}$, where $\psi(t) = U(t)\psi$. Since $D(H)$ is invariant under $U(t)$, the vector $\psi(t) = U(t)\psi$ satisfies the time-dependent Schrodinger equation

$$i\hbar\frac{d\psi}{dt} = H\psi \tag{1.12}$$

with the initial condition $\psi(0) = \psi$.

Definition. A state $M \in \mathscr{S}$ is called stationary for a quantum system with Hamiltonian H if in Schrodinger's picture

$$\frac{dM(t)}{dt} = 0$$

The state M is stationary if and only if $[M, U(t)] = 0$ for all t, and by Proposition 1.2 this is equivalent to

$$\{H, M\}_\hbar = 0,$$

in agreement with (1.11). The following simple result is fundamental.

Lemma 1.3. The pure state $M = P_\psi$ is stationary if and only if ψ is an eigenvector for H,

$$H\psi = \lambda\psi,$$

and in this case

$$\psi(t) = e^{-\frac{i}{\hbar}\lambda t}\psi$$

Proof. It follows from $U(t)P_\psi = P_\psi U(t)$ that ψ is a common eigenvector for unitary operators $U(t)$ for all $t, U(t)\psi = c(t)\psi, |c(t)| = 1$. Since $U(t)$ is a strongly continuous one-parameter group of unitary operators, the continuous function $c(t) = (U(t)\psi, \psi)$ satisfies the equation $c(t_1 + t_2) = c(t_1)\, c(t_2)$ for all $t_1, t_2 \in \mathbb{R}$, so that $c(t) = e^{-\frac{i}{\hbar}\lambda t}$ for some $\lambda \in \mathbb{R}$. Thus by Stone's theorem $\psi \in D(H)$ and $H\psi = \lambda\psi$.

In physics terminology, the eigenvectors of H are called bound states. The corresponding eigenvalues are called energy levels and are usually denoted by E. The eigenvalue equation $H\psi = E\psi$ is called the stationary Schrodinger equation.

Problem 1.5. Show that if an observable A is such that for every state M the expectation value $\langle A|M(t)\rangle$ does not depend on t, then A is a quantum integral of motion. (This is the definition of integrals of motion in the Schrodinger picture.)

Problem 1.6. Show that a solution of the initial value problem for the timedependent Schrodinger equation (1.12) is given by

$$\psi(t) = \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar}t\lambda} d\mathrm{P}(\lambda)\psi$$

where $\mathrm{P}(\lambda)$ is the resolution of identity for the Hamiltonian H.

Problem 1.7. Let D be a linear subspace of $\mathscr{H}$, consisting of Grding vectors

$$\psi_f = \int_{-\infty}^{\infty} f(s)U(s)\psi ds, \quad f \in \mathscr{S}(\mathbb{R}), \quad \psi \in \mathscr{H}$$

where $\mathscr{S}(\mathbb{R})$ is the Schwartz space of rapidly decreasing functions on $\mathbb{R}$. Prove that D is dense in $\mathscr{H}$ and is invariant for $U(t)$ and for the Hamiltonian H. (Hint: Show that $U(t)\psi_f = \psi_{f_t} \in D$, where $f_t(s) = f(s - t)$, and deduce $H\psi_f = \frac{\hbar}{i}\psi_{f'}$.)

3.1.2 Axioms of QM: Extra Discussion

(write some ideas from some fundamental articles and from section before. again: what are they? why exactly they are as they are? this is the goal of this section)

3.1.3 Heisenberg Equations

Formalism of Heisenberg equations

(main theory)

Conceptual questions about formalism of Heisenberg equations

What does one mean if one says "dynamics of observable"?

(I am not sure)

Overview of applications of Heisenberg equations

Density matrix and open quantum systems are described by Heisenberg equations

(write that this is very used there with some short examples)
(??? by the way, I don't know, why Schrodinger's one isn't used there??? there should be a reason for it)

(??? what in QFT) is described by Heisenberg equations

(I heard about it, I don't know now)

3.2 Typical Quantization

3.2.1 2. Quantization: Basic Method

To study the quantum system one needs to describe its Hilbert space of states $\mathscr{H}$ and the Hamiltonian H - a self-adjoint operator in $\mathscr{H}$ which defines the evolution of a system. When the quantum system has a classical analog, the procedure of constructing the corresponding Hilbert space $\mathscr{H}$ and the Hamiltonian H is called quantization.

Definition of quantization

Quantization of a classical system $((\mathscr{M},\{\}),,H_c)$ with the Hamiltonian function [14]H_c is a one-to-one mapping $\mathrm{Q}_\hbar : \mathcal{A} \to \mathscr{A}$ from the set of classical observables $\mathcal{A} = C^\infty(\mathscr{M})$ to the set $\mathscr{A}$ of quantum observables - the set of self-adjoint operators on a Hilbert space $\mathscr{H}$. The map $\mathrm{Q}_\hbar$ depends on the parameter $\hbar > 0$, and its restriction to the subspace of bounded classical observables $\mathcal{A}_0$ is a linear mapping to the subspace $\mathscr{A}_0$ of bounded quantum observables, which satisfies the properties

$$\lim_{\hbar\to 0} \frac{1}{2}\mathrm{Q}_\hbar^{-1}\left(\mathrm{Q}_\hbar\left(f_1\right)\mathrm{Q}_\hbar\left(f_2\right)+\mathrm{Q}_\hbar\left(f_2\right)\mathrm{Q}_\hbar\left(f_1\right)\right)=f_1 f_2$$

and

$$\lim_{\hbar\to 0} \mathrm{Q}_\hbar^{-1}\left(\left\{\mathrm{Q}_\hbar\left(f_1\right),\mathrm{Q}_\hbar\left(f_2\right)\right\}_\hbar\right)=\{f_1,f_2\} \qquad \text{for all} \qquad f_1,f_2\in\mathcal{A}_0$$

The latter property is the celebrated correspondence principle of Niels Bohr. In particular, $H_\mathrm{c} \mapsto \mathrm{Q}_\hbar\left(H_\mathrm{c}\right) = H$ - the Hamiltonian operator for a quantum system.
Remark. In physics literature the correspondence principle is often stated in the form

$$[,] \simeq \frac{\hbar}{i}\{,\} \qquad \text{as} \qquad \hbar\to 0$$

Quantum mechanics is different from classical mechanics, so that the correspondence $f \mapsto \mathrm{Q}_\hbar(f)$ cannot be an isomorphism between the Lie algebras of bounded classical and quantum

[014] Notation H_c is used to distinguish the Hamiltonian function in classical mechanics from the Hamiltonian operator H in quantum mechanics.

observables with respect to classical and quantum brackets. It becomes an isomorphism only in the limit $\hbar \to 0$ when, according to the correspondence principle, quantum mechanics turns into classical mechanics. Since quantum mechanics provides a more accurate and refined description than classical mechanics, quantization of a classical system may not be unique.

Definition. Two quantizations $\mathrm{Q}_\hbar^{(1)}$ and $\mathrm{Q}_\hbar^{(2)}$ of a given classical system $((\mathscr{M}, \{\}), , H_c)$ are said to be equivalent if there exists a linear mapping $\mathscr{U}_\hbar : \mathcal{A} \to \mathcal{A}$ such that $\mathrm{Q}_\hbar^{(2)} = \mathrm{Q}_\hbar^{(1)} \circ \mathscr{U}_\hbar$ and $\lim_{\hbar \to 0} \mathscr{U}_\hbar = \mathrm{id}$.

For many "real world" quantum systems - the systems describing actual physical phenomena - the corresponding Hamiltonian H does not depend on a choice of equivalent quantization, and is uniquely determined by the classical Hamiltonian function H_c.

2.1. Heisenberg commutation relations.

The simplest classical system with one degree of freedom is described by the phase space $\mathbb{R}^2$ with coordinates p, q and the Poisson bracket $\{,\}, associatedwiththecanonical$ symplectic form $\omega = dp \wedge dq$. In particular, the Poisson bracket between classical observables p and q - momentum and coordinate of a particle has the following simple form:

$$\{p, q\} = 1 \tag{2.1}$$

It is another postulate of quantum mechanics that under quantization classical observables p and q correspond to quantum observables P and Q -self-adjoint operators on a Hilbert space $\mathscr{H}$, satisfying the following properties.

CR1. There is a dense linear subset $D \subset \mathscr{H}$ such that $P : D \to D$ and $Q : D \to D$.
CR2. For all $\psi \in D$,

$$(PQ - QP)\psi = -i\hbar\psi$$

CR3. Every bounded operator on $\mathscr{H}$ which commutes with P and Q is a multiple of the identity operator I.

Property CR2 is called the Heisenberg commutation relation for one degree of freedom. In terms of the quantum bracket (1.6) it takes the form

$$\{P, Q\}_\hbar = I, \tag{2.2}$$

which is exactly the same as the Poisson bracket (2.1). Property CR3 is a quantum analog of the classical property that the Poisson manifold $(\mathbb{R}^2, \{\},)$ is non-degenerate: every function which Poisson commutes with p and q is a constant (see the last remark in Section 2.7 of Chapter 1).

The operators P and Q are called, respectively, the momentum operator and the coordinate operator. The correspondence $p \mapsto P, q \mapsto Q$ with P and Q satisfying CR1-CR3 is the cornerstone for the quantization of classical systems. The validity of (2.2), as well as of quantum mechanics as a whole, is confirmed by the agreement of the theory with numerous experiments.

Remark. It is tempting to extend the correspondence $p \mapsto P, q \mapsto Q$ to all observables by defining the mapping $f(p, q) \mapsto f(P, Q)$. However, this approach to quantization is rather naive: operators P and Q satisfy (2.2) and do not commute, so that one needs to understand how $f(P, Q)$

- a "function of non-commuting variables" - is actually defined. We will address this problem of the ordering of non-commuting operators P and Q in Section 3.3.

It follows from Heisenberg's uncertainty relations (see Proposition 1.4), that for any pure state $M = P_\psi$ with $\psi \in D$,

$$\sigma_M(P)\sigma_M(Q) \geq \frac{\hbar}{2}$$

This is a fundamental result saying that it is impossible to measure the coordinate and the momentum of a quantum particle simultaneously: the more accurate the measurement of one quantity is, the less accurate the value of the other is. It is often said that a quantum particle has no observed path, so that "quantum motion" differs dramatically from the motion in classical mechanics.

It is now straightforward to consider a classical system with n degrees of freedom, described by the phase space $\mathbb{R}^{2n}$ with coordinates $\boldsymbol{p} = (p_1, ..., p_n)$ and $\boldsymbol{q} = (q^1, ..., q^n)$, and the Poisson bracket $\{,\}, associatedwiththe$ canonical symplectic form $\omega = d\boldsymbol{p} \wedge d\boldsymbol{q}$. The Poisson brackets between classical observables $\boldsymbol{p}$ and $\boldsymbol{q}$ - momenta and coordinates of a particle - have the form

$$\{p_k, p_l\} = 0, \quad \left\{q^k, q^l\right\} = 0, \quad \left\{p_k, q^l\right\} = \delta_k^l, \quad k, l = 1, ..., n. \tag{2.3}$$

Corresponding momenta and coordinate operators $\boldsymbol{P} = (P_1, ..., P_n)$ and $\boldsymbol{Q} = (Q^1, ..., Q^n)$ are self-adjoint operators that have a common invariant dense linear subset $D \subset \mathscr{H}$, and on D satisfy the following commutation relations:

$$\{P_k, P_l\}_\hbar = 0, \quad \left\{Q^k, Q^l\right\}_\hbar = 0, \quad \left\{P_k, Q^l\right\}_\hbar = \delta_k^l I, \quad k, l = 1, ..., n. \tag{2.4}$$

These relations are called Heisenberg commutation relations for n degrees of freedom. The analog of CR3 is the property that every bounded operator on $\mathscr{H}$ which commutes with all operators $\boldsymbol{P}$ and $\boldsymbol{Q}$ is a multiple of the identity operator I.

The fundamental algebraic structure associated with Heisenberg commutation relations is the so-called Heisenberg algebra.

Definition. The Heisenberg algebra $\mathfrak{h}_n$ with n degrees of freedom is a Lie algebra with the generators $e^1, ..., e^n, f_1, ..., f_n, c$ and the relations

$$\left[e^k, c\right] = 0, \quad [f_k, c] = 0, \quad \left[e^k, f_l\right] = \delta_l^k c, \quad k, l = 1, ..., n \tag{2.5}$$

The invariant definition is the following. Let (V, ω) be a $2n$-dimensional symplectic vector space considered as an abelian Lie algebra, and let $\mathfrak{g}$ be a one-dimensional central extension of V by a Lie algebra 2-cocycle given by the bilinear form ω. This means that there is an exact sequence of vector spaces

$$0 \to \mathbb{R} \to \mathfrak{g} \to V \to 0 \tag{2.6}$$

and the Lie bracket in $\mathfrak{g}$ is defined by

$$[x, y] = \omega(\bar{x}, \bar{y})c \tag{2.7}$$

where $\bar{x}, \bar{y}$ are the images in V of elements $x, y \in \mathfrak{g}$, and c is the image of 1 under the embedding $\mathbb{R} \hookrightarrow \mathfrak{g}$, called the central element of $\mathfrak{g}$. A choice of a symplectic basis $e^1, ..., e^n, f_1, ..., f_n$ for V (see Section 2.6 of Chapter 1) establishes the isomorphism $\mathfrak{g} \simeq \mathfrak{h}_n$, and relations (2.5) are obtained from the Lie bracket (2.7).

By Ado's theorem, the Heisenberg algebra $\mathfrak{h}_n$ is isomorphic to a Lie subalgebra of a matrix algebra over $\mathbb{R}$. Explicitly, it is realized as a nilpotent subalgebra of the Lie algebra $\mathfrak{gl}_{n+2}$ of $(n+2) \times (n+2)$ matrices with the elements

$$\sum_{k=1}^{n}\left(u^k f_k + v_k e^k\right) + \alpha c = \begin{pmatrix} 0 & u^1 & u^2 & ... & u^n & \alpha \\ 0 & 0 & 0 & \cdots & 0 & v_1 \\ 0 & 0 & 0 & \cdots & 0 & v_2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & v_n \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix} \tag{2.8}$$

Remark. The faithful representation $\mathfrak{h}_n \to \mathfrak{gl}_{n+2}$, given by (2.8), is clearly reducible: the subspace $V = \{\boldsymbol{x} = (x_1, ..., x_{n+2}) \in \mathbb{R}^{n+2} : x_{n+2} = 0\}$ is an invariant subspace for $\mathfrak{h}_n$ with the central element c acting by zero. However, this representation is not decomposable: the vector space $\mathbb{R}^{n+2}$ cannot be written as a direct sum of V and a one-dimensional invariant subspace for $\mathfrak{h}_n$. This explains why the central element c is not represented by a diagonal matrix with the first $n+1$ zeros, but rather has a special form given by (2.8).

Analytically, Heisenberg commutation relations (2.5) correspond to an irreducible unitary representation of the Heisenberg Lie algebra $\mathfrak{h}_n$. Recall that a unitary representation ρ of $\mathfrak{h}_n$ in the Hilbert space $\mathscr{H}$ is the linear mapping $\rho : \mathfrak{h}_n \to i\mathscr{A}$ - the space of skew-Hermitian operators in $\mathscr{H}$ such that all self-adjoint operators $i\rho(x), x \in \mathfrak{h}_n$, have a common invariant dense linear subset $D \subset \mathscr{H}$ and satisfy

$$\rho([x,y])\varphi = (\rho(x)\rho(y) - \rho(y)\rho(x))\varphi, \quad x, y \in \mathfrak{h}_n, \varphi \in D.$$

Formally applying Schur's lemma we say that the representation ρ is irreducible if every bounded operator which commutes with all operators $i\rho(x)$ is a multiple of the identity operator I. Then Heisenberg commutation relations (2.5) define an irreducible unitary representation ρ of the Heisenberg Lie algebra $\mathfrak{h}_n$ in the Hilbert space $\mathscr{H}$ by setting

$$\rho\left(f_k\right) = -iP_k, \quad \rho\left(e^k\right) = -iQ^k, \quad k = 1, ..., n, \quad \rho(c) = -i\hbar I. \tag{2.9}$$

Since the operators P^k and Q_k are necessarily unbounded (see Problem 2.1), the condition

$$P_k P_l \varphi = P_l P_k \varphi \quad \text{for all} \quad \varphi \in D$$

does not necessarily imply (see Problem 2.2) that self-adjoint operators P_k and P_l commute in the sense of the definition in Section 1.1. To avoid such "pathological" representations, we will assume that ρ is an integrable representation, i.e., it can be integrated (in a precise sense specified below) to an irreducible unitary representation of the Heisenberg group $\mathbf{H}_n$ – a connected, simply-connected Lie group with the Lie algebra $\mathfrak{h}_n$.

Explicitly, the Heisenberg group is a unipotent subgroup of the Lie algebra $\mathrm{SL}(n+2, \mathbb{R})$ with the elements

$$g = \begin{pmatrix} 1 & u^1 & u^2 & \cdots & u^n & \alpha \\ 0 & 1 & 0 & \cdots & 0 & v_1 \\ 0 & 0 & 1 & \cdots & 0 & v_2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & v_n \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{pmatrix}.$$

The exponential map $\exp : \mathfrak{h}_n \to \mathbf{H}_n$ is onto, and the Heisenberg group $\mathbf{H}_n$ is generated by two n-parameter abelian subgroups

$$\exp \boldsymbol{u}X = \exp\left(\sum_{k=1}^{n} u^k f_k\right), \quad \exp \boldsymbol{v}Y = \exp\left(\sum_{k=1}^{n} v_k e^k\right), \quad \boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^n$$

and a one-parameter center $\exp \alpha c$, which satisfy the relations

$$\exp \boldsymbol{u}X \exp \boldsymbol{v}Y = \exp(-\boldsymbol{u}\boldsymbol{v}c) \exp \boldsymbol{v}Y \exp \boldsymbol{u}X, \quad \boldsymbol{u}\boldsymbol{v} = \sum_{k=0}^{n} u^k v_k \tag{2.10}$$

Indeed, it follows from (2.5) that $[\boldsymbol{u}X, \boldsymbol{v}Y] = -\boldsymbol{u}\boldsymbol{v}\boldsymbol{c}$ is a central element, so that using the Baker-Campbell-Hausdorff formula we obtain

$$\exp \boldsymbol{u}X \exp \boldsymbol{v}Y = \exp\left(-\frac{1}{2}\boldsymbol{u}\boldsymbol{v}c\right) \exp(\boldsymbol{u}X + \boldsymbol{v}Y)$$
$$\exp \boldsymbol{v}Y \exp \boldsymbol{u}X = \exp\left(\frac{1}{2}\boldsymbol{u}\boldsymbol{v}\boldsymbol{c}\right) \exp(\boldsymbol{u}X + \boldsymbol{v}Y)$$

In the matrix realization, the exponential map is given by the matrix exponential and we get $e^{uX} = I + \boldsymbol{u}X, e^{\boldsymbol{v}Y} = I + \boldsymbol{v}Y$, and $e^{\alpha c} = I + \alpha c$, where I is the $(n+2) \times (n+2)$ identity matrix.

Let R be an irreducible unitary representation of the Heisenberg group $\mathbf{H}_n$ in the Hilbert space $\mathscr{H}$ - a strongly continuous group homomorphism $R : \mathbf{H}_n \to \mathscr{U}(\mathscr{H})$, where $\mathscr{U}(\mathscr{H})$ is the group of unitary operators in $\mathscr{H}$. By Schur's lemma, $R(e^{\alpha c}) = e^{-i\lambda\alpha} I, \lambda \in \mathbb{R}$. Suppose now that $\lambda = \hbar$, and define two strongly continuous n-parameter abelian groups of unitary operators

$$U(\boldsymbol{u}) = R(\exp \boldsymbol{u}X), \quad V(\boldsymbol{v}) = R(\exp \boldsymbol{v}Y), \quad \boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^n$$

Then it follows from (2.10) that unitary operators $U(\boldsymbol{u})$ and $V(\boldsymbol{v})$ satisfy commutation relations

$$U(\boldsymbol{u})V(\boldsymbol{v}) = e^{i\hbar\boldsymbol{u}\boldsymbol{v}} V(\boldsymbol{v})U(\boldsymbol{u}) \tag{2.11}$$

called Weyl relations. Let $\boldsymbol{P} = (P_1, ..., P_n)$ and $\boldsymbol{Q} = (Q^1, ..., Q^n)$ be, respectively, infinitesimal generators of the subgroups $U(\boldsymbol{u})$ and $V(\boldsymbol{v})$, given by the Stone theorem,

$$P_k = i\frac{\partial U(\boldsymbol{u})}{\partial u^k}\bigg|_{\boldsymbol{u}=0} \quad \text{and} \quad Q^k = i\frac{\partial V(\boldsymbol{v})}{\partial v_k}\bigg|_{\boldsymbol{v}=0}, \quad k = 1, ..., n.$$

Taking the second partial derivatives of Weyl relations (2.11) at the origin $\boldsymbol{u} = \boldsymbol{v} = 0$ and using the solution of Problem 1.7 in the previous section, we easily obtain the following result.

Lemma 2.1. Let $R : \mathbf{H}_n \to \mathscr{U}(\mathscr{H})$ be an irreducible unitary representation of the Heisenberg group $\mathbf{H}_n$ in $\mathscr{H}$ such that $R(e^{\alpha c}) = e^{-i\hbar\alpha} I$, and let $\boldsymbol{P} = (P_1, ..., P_n)$ and $\boldsymbol{Q} = (Q^1, ..., Q^n)$ be, respectively, infinitesimal generators of the strongly continuous n-parameter abelian subgroups $U(\boldsymbol{u})$ and $V(\boldsymbol{v})$.

Then formulas (2.9) define an irreducible unitary representation ρ of the Heisenberg algebra $\mathfrak{h}_n$ in $\mathscr{H}$.

The representation ρ in Lemma 2.1 is called the differential of a representation R, and is denoted by dR. The irreducible unitary representation ρ of $\mathfrak{h}_n$ is called integrable if $\rho = dR$ for some irreducible unitary representation R of $\mathbf{H}_n$.

Remark. Not every irreducible unitary representation of the Heisenberg algebra is integrable, so that Weyl relations cannot be obtained from the Heisenberg commutation relations. However, the following heuristic argument (which ignores the subtleties of dealing with unbounded operators) is commonly used in physics textbooks. Consider the case of one degree of freedom and start with

$$\{P, Q\}_\hbar = I.$$

Since the quantum bracket satisfies the Leibniz rule we have, for a "suitable" function f,

$$\{f(P), Q\}_h = f'(P).$$

In particular, choosing $f(P) = e^{-iuP} = U(u)$, we obtain

$$U(u)Q - QU(u) = \hbar u U(u) \quad \text{or} \quad U(u)QU(u)^{-1} = Q + \hbar u I.$$

This implies, for a "suitable" function g,

$$U(u)g(Q) = g(Q + \hbar u I)U(u),$$

and setting $g(Q) = e^{-ivQ} = V(v)$, we get the Weyl relation.
We will prove in Section 3.1 that all integrable irreducible unitary representations of the Heisenberg algebra $\mathfrak{h}_n$ with the same action of the central element c are unitarily equivalent. This justifies the following mathematical formulation of the Heisenberg commutation relations for n degrees of freedom.

A9 (Heisenberg's Commutation Relations). Momenta and coordinate operators $\boldsymbol{P} = (P_1, ..., P_n)$ and $\boldsymbol{Q} = (Q^1, ..., Q^n)$ for a quantum particle with n degrees of freedom are defined by formulas (2.9), where ρ is an integrable irreducible unitary representation of the Heisenberg algebra $\mathfrak{h}_n$ with the property $\rho(c) = -i\hbar I$.

Problem 2.1. Prove that there are no bounded operators on the Hilbert space $\mathscr{H}$ satisfying $[A, B] = I$.

Problem 2.2. Give an example of self-adjoint operators A and B which have a common invariant dense linear subset $D \subset \mathscr{H}$ such that $AB\varphi = BA\varphi$ for all $\varphi \in D$, but e^{iA} and e^{iB} do not commute.

Problem 2.3. Prove Lemma 2.1. (Hint: As in Problem 1.7, let D be the linear set of Grding vectors

$$\psi_f = \int_{\mathbb{R}^{2n}} f(\boldsymbol{u}, \boldsymbol{v}) U(\boldsymbol{u}) V(\boldsymbol{v}) \psi d^n\boldsymbol{u} d^n\boldsymbol{v}, \quad f \in \mathscr{S}\left(\mathbb{R}^{2n}\right), \psi \in \mathscr{H}$$

where $\mathscr{S}(\mathbb{R}^{2n})$ is the Schwartz space of rapidly decreasing functions on $\mathbb{R}^{2n}$.)

2.2. Coordinate and momentum representations.

We start with the case of one degree of freedom and consider two natural realizations of the Heisenberg commutation relation. They are defined by the property that one of the self-adjoint operators P and Q is "diagonal" (i.e., is a multiplication by a function operator in the corresponding Hilbert space).

In the coordinate representation, $\mathscr{H} = L^2(\mathbb{R}, dq)$ is the L^2-space on the configuration space $\mathbb{R}$ with the coordinate q, which is a Lagrangian subspace of $\mathbb{R}^2$ defined by the equation $p = 0$. Set

$$D(Q) = \left\{ \varphi \in \mathscr{H} : \int_{-\infty}^{\infty} q^2 |\varphi(q)|^2 dq < \infty \right\}$$

and for $\varphi \in D(Q)$ define the operator Q as a "multiplication by q operator",

$$(Q\varphi)(q) = q\varphi(q), q \in \mathbb{R}$$

justifying the name coordinate representation. The coordinate operator Q is obviously self-adjoint and its projection-valued measure is given by

$$(\mathrm{P}(E)\varphi)(q) = \chi_E(q)\varphi(q) \tag{2.12}$$

where χ_E is the characteristic function of a Borel subset $E \subseteq \mathbb{R}$. Therefore $\operatorname{supp} \mathbf{P} = \mathbb{R}$ and $\sigma(Q) = \mathbb{R}$.

Recall that a self-adjoint operator A has an absolutely continuous spectrum if for every $\psi \in \mathscr{H}, \|\psi\| = 1$, the probability measure ν_ψ,

$$\nu_\psi(E) = (\mathrm{P}_A(E)\psi, \psi), \quad E \in \mathscr{B}(\mathbb{R})$$

is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}$.

Lemma 2.2. The coordinate operator Q has an absolutely continuous spectrum $\mathbb{R}$, and every bounded operator B which commutes with Q is a function of $Q, B = f(Q)$ with $f \in L^\infty(\mathbb{R})$.

Proof. It follows from (2.12) that $\nu_\psi(E) = \int_E |\psi(q)|^2 dq$, which proves the first statement. Now a bounded operator B on $\mathscr{H}$ commutes with Q if and only if $B\mathrm{P}(E) = \mathrm{P}(E)B$ for all $E \in \mathscr{B}(\mathbb{R})$, and using (2.12) we get

$$B(\chi_E\varphi) = \chi_E B(\varphi) \tag{2.13}$$

Choosing in (2.13) $E = E_1$ and $\varphi = \chi_{E_2}$, where E_1 and E_2 have finite Lebesgue measure, we obtain

$$B(\chi_{E_1} \cdot \chi_{E_2}) = B(\chi_{E_1 \cap E_2}) = \chi_{E_1} B(\chi_{E_2}) = \chi_{E_2} B(\chi_{E_1}),$$

so that denoting $f_E = B(\chi_E)$ we get $\operatorname{supp} f_E \subseteq E$, and

$$f_{E_1}|_{E_1 \cap E_2} = f_{E_2}|_{E_1 \cap E_2}$$

for all $E_1, E_2 \in \mathscr{B}(\mathbb{R})$ with finite Lebesgue measure. Thus there exists a measurable function f on $\mathbb{R}$ such that $f|_E = f_E|_E$ for every $E \in \mathscr{B}(\mathbb{R})$ with finite Lebesgue measure. The linear subspace spanned by all $\chi_E \in L^2(\mathbb{R})$ is dense in $L^2(\mathbb{R})$ and the operator B is continuous, so that we get

$$(B\varphi)(q) = f(q)\varphi(q) \quad \text{for all} \quad \varphi \in L^2(\mathbb{R})$$

Since B is a bounded operator, $f \in L^\infty(\mathbb{R})$ and $\|B\| = \|f\|_\infty$.

Remark. By the Schwartz kernel theorem, the operator B can be represented by an integral operator with a distributional kernel $K(q, q')$. Then the commutativity $BQ = QB$ implies that, in the distributional sense,

$$(q - q')K(q, q') = 0,$$

so that K is "proportional" to the Dirac delta-function, i.e.,

$$K(q, q') = f(q)\delta(q - q')$$

with some $f \in L^\infty(\mathbb{R})$. This argument is usually given in the physics textbooks.

Remark. The operator Q has no eigenvectors - the eigenvalue equation

$$Q\varphi = \lambda\varphi$$

has no solutions in $L^2(\mathbb{R})$. However, in the distributional sense, this equation for every $\lambda \in \mathbb{R}$ has a unique (up to a constant factor) solution $\varphi_\lambda(q) = \delta(q - \lambda)$, and these "generalized eigenfunctions", also called eigenfunctions of the continuous spectrum, combine to a Schwarz kernel of the identity operator I on $L^2(\mathbb{R})$. This reflects the fact that operator Q is diagonal in the coordinate representation.

Remark. Normalization of the eigenfunctions of the continuous spectrum $\varphi_\lambda(q)$ can be also determined by the condition that for every $\lambda \in \mathbb{R}$ the function

$$\Phi_\lambda(q) = \int_{\lambda_0}^{\lambda} \varphi_\mu(q) d\mu, \quad \Phi_\lambda \in L^2(\mathbb{R})$$

satisfies

$$\lim_{\Delta \to 0} \frac{1}{\Delta} \|\Phi_{\lambda+\Delta} - \Phi_\lambda\|^2 = 1 \tag{2.14}$$

Here $\lambda_0 \in \mathbb{R}$ is fixed and does not enter (2.14). Indeed, in our case $\Phi_\lambda = \chi_{(\lambda_0,\lambda)}$ - the characteristic function of the interval (λ_0, λ) - so that $\|\Phi_{\lambda+\Delta^-} \Phi_\lambda\|^2 = \Delta$.

For a pure state $M = P_\psi, \|\psi\| = 1$, the corresponding probability measure μ_Q on $\mathbb{R}$ is given by

$$\mu_Q(E) = \nu_\psi(E) = \int_E |\psi(q)|^2 dq, \quad E \in \mathscr{B}(\mathbb{R})$$

Physically, this is interpreted that in the state P_ψ with the "wave function" $\psi(q)$, the probability of finding a quantum particle between q and $q + dq$ is $|\psi(q)|^2 dq$. In other words, the modulus square of a wave function is the probability distribution for the coordinate of a quantum particle.

The corresponding momentum operator P is given by a differential operator

$$P = \frac{\hbar}{i} \frac{d}{dq}$$

with $D(P) = W^{1,2}(\mathbb{R})$ - the Sobolev space of absolutely continuous functions f on $\mathbb{R}$ such that f and its derivative f' (defined a.e.) are in $L^2(\mathbb{R})$. The operator P is self-adjoint and it is straightforward to verify that on $D = C_c^\infty(\mathbb{R})$, the space of smooth functions on $\mathbb{R}$ with compact support,

$$QP - PQ = i\hbar I$$

Remark. The operator P on $\mathscr{H}$ has no eigenvectors - the eigenvalue equation

$$P\varphi = p\varphi, p \in \mathbb{R}$$

has a solution

$$\varphi(q) = \text{ const } \times e^{\frac{i}{\hbar} pq}$$

which does not belong to $L^2(\mathbb{R})$. We will see later that the family of normalized eigenfunctions of the continuous spectrum

$$\varphi_p(q) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} pq}$$

combines to a Schwartz kernel of the inverse $\hbar$-dependent Fourier transform operator, which diagonalizes the momentum operator P. In the distributional sense,

$$\int_{-\infty}^{\infty} \varphi_p(q) \overline{\varphi_{p'}(q)} dq = \delta(p - p')$$

Remark. As for the case of the coordinate operator, the normalization of the eigenfunctions of the continuous spectrum $\varphi_p(q)$ of the momentum operator can be determined from the condition (2.14). Indeed,

$$\Phi_p(q) = \int_{p_0}^{p} ce^{\frac{i}{\hbar}kq} dk = \frac{c\hbar}{iq}\left(e^{\frac{i}{\hbar}pq} - e^{\frac{i}{\hbar}p_0 q}\right)$$

so that

$$\Phi_{p+\Delta}(q) - \Phi_p(q) = \frac{2c\hbar}{q} e^{\frac{i}{\hbar}(p+\frac{1}{2}\Delta)q} \sin\frac{\Delta q}{2\hbar}.$$

Using the elementary integral, we obtain

$$\frac{1}{\Delta}\left\|\Phi_{p+\Delta}(q) - \Phi_p(q)\right\|^2 = 2c^2\hbar \int_{-\infty}^{\infty} \frac{\sin^2 q}{q^2} dq = 2\pi c^2\hbar$$

so that $c = \frac{1}{\sqrt{2\pi\hbar}}$.

Proposition 2.1. The coordinate representation defines an irreducible, unitary, integrable representation of the Heisenberg algebra.

Proof. To show that the coordinate representation is integrable, let $U(u) = e^{-iuP}$ and $V(v) = e^{-ivQ}$ be the corresponding one-parameter groups of unitary operators. Clearly, $(V(v)\varphi)\psi(q) = e^{-ivq}\varphi(q)$ and it easily follows from the Stone theorem (or by the definition of a derivative) that $(U(u)\varphi)(q) = \varphi(q - \hbar u)$, so that unitary operators $U(u)$ and $V(v)$ satisfy the Weyl relation (2.11). Such a realization of the Weyl relation is called the Schrodinger representation.

To prove that the coordinate representation is irreducible, let B be a bounded operator commuting with P and Q. By Lemma 2.2, $T = f(Q)$ for some $f \in L^\infty(\mathbb{R})$. Now commutativity between T and P implies that

$$TU(u) = U(u)T \quad \text{for all} \quad u \in \mathbb{R},$$

which is equivalent to $f(q - \hbar u) = f(q)$ for all $q, u \in \mathbb{R}$, so that $f = \text{const}$ a.e. on $\mathbb{R}$.

To summarize, the coordinate representation is characterized by the property that the coordinate operator Q is a multiplication by q operator and the momentum operator P is a differentiation operator,

$$Q = q \quad \text{and} \quad P = \frac{\hbar}{i}\frac{d}{dq}.$$

Similarly, momentum representation is defined by the property that the momentum operator P is a multiplication by p operator. Namely let $\mathscr{H} = L^2(\mathbb{R}, dp)$ be the Hilbert L^2-space on the "momentum space" $\mathbb{R}$ with the coordinate p, which is a Lagrangian subspace of $\mathbb{R}^2$ defined by the equation $q = 0$. The coordinate and momentum operators are given by

$$\hat{Q} = i\hbar\frac{d}{dp} \quad \text{and} \quad \hat{P} = p$$

and satisfy the Heisenberg commutation relation. As the coordinate representation, the momentum representation is an irreducible, unitary, integrable representation of the Heisenberg algebra. In the momentum representation, the modulus square of the wave function $\psi(p)$ of a pure state $M = P_\psi$,
$\|\psi\| = 1$, is the probability distribution for the momentum of the quantum particle, i.e., the probability that a quantum particle has momentum between p and $p + dp$ is $|\psi(p)|^2 dp$.

Let $\mathscr{F}_\hbar : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ be the $\hbar$-dependent Fourier transform operator, defined by

$$\hat{\varphi}(p) = \mathscr{F}_\hbar(\varphi)(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar}pq}\varphi(q) dq$$

Here the integral is understood as the limit $\hat{\varphi} = \lim_{n\to\infty} \hat{\varphi}_n$ in the strong topology on $L^2(\mathbb{R})$, where

$$\hat{\varphi}_n(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-n}^{n} e^{-\frac{i}{\hbar}pq} \varphi(q) dq$$

By Plancherel's theorem, $\mathscr{F}_\hbar$ is a unitary operator on $L^2(\mathbb{R})$,

$$\mathscr{F}_\hbar \mathscr{F}_\hbar^* = \mathscr{F}_\hbar^* \mathscr{F}_\hbar = I,$$

and

$$\hat{Q} = \mathscr{F}_\hbar Q \mathscr{F}_\hbar^{-1}, \quad \hat{P} = \mathscr{F}_\hbar P \mathscr{F}_\hbar^{-1}$$

so that coordinate and momentum representations are unitarily equivalent. In particular, since the operator $\hat{P}$ is obviously self-adjoint, this immediately shows that the operator P is self-adjoint.

For n degrees of freedom, the coordinate representation is defined by setting $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$, where $d^n\boldsymbol{q} = dq^1 \cdots dq^n$ is the Lebesgue measure on $\mathbb{R}^n$, and

$$\boldsymbol{Q} = \boldsymbol{q} = \left(q^1, ..., q^n\right), \quad \boldsymbol{P} = \frac{\hbar}{i}\frac{\partial}{\partial \boldsymbol{q}} = \left(\frac{\hbar}{i}\frac{\partial}{\partial q^1}, ..., \frac{\hbar}{i}\frac{\partial}{\partial q^n}\right)$$

Here $\mathbb{R}^n$ is the configuration space with coordinates $\boldsymbol{q}$ - a Lagrangian subspace of $\mathbb{R}^{2n}$ defined by the equations $\boldsymbol{p} = 0$. The coordinate and momenta operators are self-adjoint and satisfy Heisenberg commutation relations. Projection-valued measures for the operators Q^k are given by

$$\left(\mathrm{P}_k(E)\varphi\right)(\boldsymbol{q}) = \chi_{\lambda_k^{-1}(E)}(\boldsymbol{q})\varphi(\boldsymbol{q})$$

where $E \in \mathscr{B}(\mathbb{R})$ and $\lambda_k : \mathbb{R}^n \to \mathbb{R}$ is a canonical projection onto the k-th component, $k = 1, ..., n$. Correspondingly, the projection-valued measure P for the commutative family $\boldsymbol{Q} = (Q^1, ..., Q^n)$ (see Proposition 1.3) is defined on the Borel subsets $\boldsymbol{E} \subseteq \mathbb{R}^n$ by

$$(\mathrm{P}(\boldsymbol{E})\varphi)(\boldsymbol{q}) = \chi_{\boldsymbol{E}}(\boldsymbol{q})\varphi(\boldsymbol{q})$$

The family Q has absolutely continuous joint spectrum $\mathbb{R}^n$.
Coordinate operators $Q^1, ..., Q^n$ form a complete system of commuting observables. This means, by definition, that none of these operators is a function of the other operators, and that every bounded operator commuting with $Q^1, ..., Q^n$ is a function of $Q^1, ..., Q^n$, i.e., is a multiplication by $f(\boldsymbol{q})$
operator for some $f \in L^\infty(\mathbb{R}^n)$. The proof repeats verbatim the proof of Lemma 2.2. For a pure state $M = P_\psi, \|\psi\| = 1$, the modulus square $|\psi(\boldsymbol{q})|^2$ of the wave function is the density of a joint distribution function $\mu_{\boldsymbol{Q}}$ for the commutative family $\boldsymbol{Q}$, i.e., the probability of finding a quantum particle in a Borel subset $E \subseteq \mathbb{R}^n$ is given by

$$\mu_{\boldsymbol{Q}}(\boldsymbol{E}) = \int_{\boldsymbol{E}} |\psi(\boldsymbol{q})|^2 d^n\boldsymbol{q}.$$

The coordinate representation defines an irreducible, unitary, integrable representation of the Heisenberg algebra $\mathfrak{h}_n$. Indeed, n-parameter groups of unitary operators $U(\boldsymbol{u}) = e^{-i\boldsymbol{u}\boldsymbol{P}}$ and $V(\boldsymbol{v}) = e^{-i\boldsymbol{v}\boldsymbol{Q}}$ are given by

$$(U(\boldsymbol{u})\varphi)(\boldsymbol{q}) = \varphi(\boldsymbol{q} - \hbar\boldsymbol{u}), \quad (V(\boldsymbol{v})\varphi)(\boldsymbol{q}) = e^{-i\boldsymbol{v}\boldsymbol{q}}\varphi(\boldsymbol{q})$$

and satisfy Weyl relations (2.11). The same argument as in the proof of Proposition 2.1 shows that this representation of the Heisenberg group $\mathbf{H}_n$, called the Schrodinger representation for n degrees of freedom, is irreducible.

In the momentum representation, $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{p})$, where $d^n\boldsymbol{p} = dp_1 \cdots dp_n$ is the Lebesgue measure on $\mathbb{R}^n$, and

$$\hat{\boldsymbol{Q}} = i\hbar\frac{\partial}{\partial \boldsymbol{p}} = \left(i\hbar\frac{\partial}{\partial p_1}, ..., i\hbar\frac{\partial}{\partial p_n}\right), \quad \hat{\boldsymbol{P}} = \boldsymbol{p} = (p_1, ..., p_n).$$

Here $\mathbb{R}^n$ is the momentum space with coordinates $\boldsymbol{p}$ - a Lagrangian subspace of $\mathbb{R}^{2n}$ defined by the equations $\boldsymbol{q} = 0$.

The coordinate and momentum representations are unitarily equivalent by the Fourier transform. As in the case $n = 1$, the Fourier transform $\mathscr{F}_\hbar$: $L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is a unitary operator defined by

$$\begin{aligned}\hat{\varphi}(\boldsymbol{p}) = \mathscr{F}_\hbar(\varphi)(\boldsymbol{p}) &= (2\pi\hbar)^{-n/2}\int_{\mathbb{R}^n} e^{-\frac{i}{\hbar}\boldsymbol{pq}}\varphi(\boldsymbol{q})d^n\boldsymbol{q} \\ &= \lim_{N\to\infty}(2\pi\hbar)^{-n/2}\int_{|\boldsymbol{q}|\le N} e^{-\frac{i}{\hbar}\boldsymbol{pq}}\varphi(\boldsymbol{q})d^n\boldsymbol{q}\end{aligned}$$

where the limit is understood in the strong topology on $L^2(\mathbb{R}^n)$. As in the case $n = 1$, we have

$$\hat{Q}_k = \mathscr{F}_\hbar Q_k \mathscr{F}_\hbar^{-1}, \quad \hat{P}_k = \mathscr{F}_\hbar P_k \mathscr{F}_\hbar^{-1}, \quad k = 1, ..., n.$$

In particular, since operators $\hat{P}_1, ..., \hat{P}_n$ are obviously self-adjoint, this immediately shows that $P_1, ..., P_n$ are also self-adjoint.

Remark. Following Dirac, physicists denote a vector $\psi \in \mathscr{H}$ by a ket vector $|\psi\rangle$, a vector $\varphi \in \mathscr{H}^*$ in the dual space to $\mathscr{H}$ ($\mathscr{H}^* \simeq \mathscr{H}$ is a complex antilinear isomorphism) by a bra vector $\langle\varphi|$, and their inner product by $\langle\varphi|\psi\rangle$. In standard mathematics notation,

$$(\psi, \varphi) = \langle\varphi|\psi\rangle \quad \text{and} \quad (A\psi, \varphi) = \langle\varphi|A|\psi\rangle,$$

where A is a linear operator. From a physics point of view, Dirac's notation is intuitive and convenient for working with coordinate and momentum representations. Denoting by $|\boldsymbol{q}\rangle = \delta(\boldsymbol{q} - \boldsymbol{q}')$ and $|\boldsymbol{p}\rangle = (2\pi\hbar)^{-n/2}e^{\frac{i}{\hbar}\boldsymbol{pq}}$ the set of generalized common eigenfunctions for the operators $\boldsymbol{Q}$ and $\boldsymbol{P}$, respectively, we formally get

$$\boldsymbol{Q}|\boldsymbol{q}\rangle = \boldsymbol{q}|\boldsymbol{q}\rangle, \quad \boldsymbol{P}|\boldsymbol{p}\rangle = \boldsymbol{p}|\boldsymbol{p}\rangle$$

where operators $\mathbf{Q}$ act on $\boldsymbol{q}'$, and

$$\begin{aligned}\langle\boldsymbol{q}|\psi\rangle &= \int_{\mathbb{R}^n}\delta(\boldsymbol{q} - \boldsymbol{q}')\,\psi(\boldsymbol{q}')\,d^n\boldsymbol{q}' = \psi(\boldsymbol{q}), \\ \langle\boldsymbol{p}|\psi\rangle &= (2\pi\hbar)^{-n/2}\int_{\mathbb{R}^n} e^{-\frac{i}{\hbar}\boldsymbol{pq}}\psi(\boldsymbol{q})d^n\boldsymbol{q} = \hat{\psi}(\boldsymbol{p}),\end{aligned}$$

as well as $\langle\boldsymbol{q}|\boldsymbol{q}'\rangle = \delta(\boldsymbol{q} - \boldsymbol{q}')$, $\langle\boldsymbol{p}|\boldsymbol{p}'\rangle = \delta(\boldsymbol{p} - \boldsymbol{p}')$. Though in our exposition we are not using Dirac's notation, these formulas would help the interested reader "translate" the notation used in physics textbooks to standard mathematics notation.

Remark. We will show in Section 3.2 that every Lagrangian subspace of the symplectic vector space $\mathbb{R}^{2n}$ with the canonical symplectic form $\omega = d\boldsymbol{p} \wedge d\boldsymbol{q}$ gives rise to an integrable, unitary, irreducible representation of the Heisenberg algebra $\mathfrak{h}_n$. This is the simplest example of the real polarization, which for a given symplectic manifold $(\mathscr{M}, \omega)$ is defined as an integrable

distribution $\{\mathscr{L}_x\}_{x\in\mathscr{M}}$ of Lagrangian subspaces $\mathscr{L}_x$ of tangent spaces $T_x\mathscr{M}$. The notion of a polarization plays a fundamental role in geometric quantization: it allows us to construct (under certain conditions) the Hilbert space of states $\mathscr{H}$ associated with the classical phase space $(\mathscr{M},\omega)$. In the linear case $\mathscr{M}=\mathbb{R}^{2n}$ every Lagrangian subspace $\mathscr{L}$ in $\mathbb{R}^{2n}$ gives rise to a real polarization by using the identification $T_x\mathbb{R}^{2n}\simeq\mathbb{R}^{2n}$. In particular, for the coordinate representation, $\mathscr{L}$ is given by the equation $\boldsymbol{q}=0$, and for the momentum representation - by the equation $\boldsymbol{p}=0$. The corresponding Hilbert $\mathscr{H}$ space consists of functions on $\mathbb{R}^{2n}$ which are constant along the fibers of the polarization.

Problem 2.4. Give an example of a non-integrable representation of the Heisenberg algebra.

Problem 2.5. Prove that there exists $\varphi\in\mathscr{H}=L^2(\mathbb{R},dq)$ such that the vectors $\mathrm{P}(E)\varphi, E\in\mathscr{B}(\mathbb{R})$, where P is a projection-valued measure for the coordinate operator Q, are dense in $\mathscr{H}$.

Problem 2.6. Find the generating operator for the commutative family $\boldsymbol{Q}=(Q^1,...,Q^n)$. Does it have a physical interpretation?

Problem 2.7. Find the projection-valued measure for the commutative family $\boldsymbol{P}=(P_1,...,P_n)$ in the coordinate representation.

3.2.2 2. Quantization: Basic Models

2.3. Free quantum particle.

A free classical particle with one degree of freedom is described by the phase space $\mathbb{R}^2$ with coordinates p,q and the Poisson bracket (2.1), and by the Hamiltonian function

$$H_{\mathrm{c}}(p,q)=\frac{p^2}{2m} \tag{2.15}$$

The Hamiltonian operator of a free quantum particle with one degree of freedom is

$$H_0=\frac{P^2}{2m}$$

and in coordinate representation is given by

$$H_0=-\frac{\hbar^2}{2m}\frac{d^2}{dq^2}$$

It is a self-adjoint operator on $\mathscr{H}=L^2(\mathbb{R},dq)$ with $D(H_0)=W^{2,2}(\mathbb{R})$ - the Sobolev space of functions in $L^2(\mathbb{R})$, whose generalized first and second derivatives are in $L^2(\mathbb{R})$.

The operator H_0 is positive with absolutely continuous spectrum $[0,\infty)$ of multiplicity two. Indeed, let $\mathfrak{H}_0=L^2(\mathbb{R}_{>0},\mathbb{C}^2;d\sigma)$ be the Hilbert space of $\mathbb{C}^2$-valued measurable functions Ψ on the semi-line $\mathbb{R}_{>0}=(0,\infty)$, which are square-integrable with respect to the measure $d\sigma(\lambda)=\sqrt{\frac{m}{2\lambda}}d\lambda$,

$$\mathfrak{H}_0=\left\{\Psi(\lambda)=\begin{pmatrix}\psi_1(\lambda)\\ \psi_2(\lambda)\end{pmatrix}:\|\Psi\|^2=\int_0^\infty\left(|\psi_1(\lambda)|^2+|\psi_2(\lambda)|^2\right)d\sigma(\lambda)<\infty\right\}.$$

It follows from the unitarity of the Fourier transform that the operator $\mathscr{U}_0:L^2(\mathbb{R},dq)\to\mathfrak{H}_0$,

$$\mathscr{U}_0(\psi)(\lambda)=\Psi(\lambda)=\begin{pmatrix}\hat{\psi}(\sqrt{2m\lambda})\\ \hat{\psi}(-\sqrt{2m\lambda})\end{pmatrix}$$

is unitary, $\mathscr{U}_0^*\mathscr{U}_0=I$ and $\mathscr{U}_0\mathscr{U}_0^*=I_0$, where I and I_0 are, respectively, identity operators in $\mathscr{H}$ and $\mathfrak{H}_0$. The operator $\mathscr{U}_0$ establishes the isomorphism $L^2(\mathbb{R},dq)\simeq\mathfrak{H}_0$, and since in the momentum representation H_0 is a multiplication by $\frac{1}{2m}p^2$ operator, the operator $\mathscr{U}_0H_0\mathscr{U}_0^{-1}$ is

a multiplication by λ operator in $\mathfrak{H}_0$.
Remark. The Hamiltonian operator H_0 has no eigenvectors - the eigenvalue equation

$$H_0\psi = \lambda\psi$$

has no solutions in $L^2(\mathbb{R})$. However, for every $\lambda = \frac{1}{2m}k^2 > 0$ this differential equation has two linear independent bounded solutions

$$\psi_k^{(\pm)}(q) = \frac{1}{\sqrt{2\pi\hbar}} e^{\pm\frac{i}{\hbar}kq}, \quad k > 0$$

In the distributional sense, these eigenfunctions of the continuous spectrum combine to a Schwartz kernel of the unitary operator $\mathscr{U}_0$, which establishes
the isomorphism between $\mathscr{H} = L^2(\mathbb{R}, dq)$ and the Hilbert space $\mathfrak{H}_0$, where H_0 acts as a multiplication by λ operator. The normalization of the eigenfunctions of the continuous spectrum is also determined by the condition (2.14):

$$\lim_{\Delta\to 0}\frac{1}{\Delta}\left\|\Psi_{k+\Delta}^{(\pm)} - \Psi_k^{(\pm)}\right\|^2 = 1, \quad \lim_{\Delta\to 0}\frac{1}{\Delta}\left(\Psi_{k+\Delta}^{(+)} - \Psi_k^{(+)}, \Psi_{k+\Delta}^{(-)} - \Psi_k^{(-)}\right) = 0$$

where $\Psi_k^{(\pm)}(q) = \int_{k_0}^k \psi_p^{(\pm)}(q)dp$.
The Cauchy problem for the Schrodinger equation for a free particle,

$$i\hbar\frac{d\psi(t)}{dt} = H_0\psi(t), \quad \psi(0) = \psi \tag{2.16}$$

is easily solved by the Fourier transform. Indeed, in the momentum representation it takes the form

$$i\hbar\frac{\partial\hat{\psi}(p,t)}{\partial t} = \frac{p^2}{2m}\hat{\psi}(p,t), \quad \hat{\psi}(p,0) = \hat{\psi}(p)$$

so that

$$\hat{\psi}(p,t) = e^{-\frac{ip^2}{2m\hbar}t}\hat{\psi}(p).$$

In the coordinate representation, the solution of (2.16) is given by

$$\psi(q,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}pq}\hat{\psi}(p,t)dp = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}\chi(p,q,t)t}\hat{\psi}(p)dp \tag{2.17}$$

where

$$\chi(p,q,t) = -\frac{p^2}{2m} + \frac{pq}{t}.$$

Formula (2.17) describes the motion of a quantum particle, and admits the following physical interpretation. Let initial condition ψ in (2.16) be such that its Fourier transform $\hat{\psi} = \mathcal{F}_\hbar(\psi)$ is a smooth function supported in a neighborhood U_0 of $p_0 \in \mathbb{R}\backslash\{0\}, 0 \notin U_0$, and

$$\int_{-\infty}^{\infty}|\hat{\psi}(p)|^2dp = 1$$

Such states are called "wave packets". Then for every compact subset $E \subset \mathbb{R}$ we have

$$\lim_{|t|\to\infty}\int_E |\psi(q,t)|^2dq = 0 \tag{2.18}$$

Since

$$\int_{-\infty}^{\infty} |\psi(q,t)|^2 dq = 1$$

for all t, it follows from (2.18) that the particle leaves every compact subset of $\mathbb{R}$ as $|t| \to \infty$ and the quantum motion is infinite. To prove (2.18), observe that the function $\chi(p,q,t)$ - the "phase" in integral representation (2.17)

- has the property that $\left|\frac{\partial \chi}{\partial p}\right| > C > 0$ for all $p \in U_0, q \in E$ and large enough $|t|$. Integrating by parts we get

$$\begin{aligned}\psi(q,t) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{U_0} e^{\frac{i}{\hbar}\chi(p,q,t)t} \hat{\psi}(p) dp \\ &= -\frac{1}{it}\sqrt{\frac{\hbar}{2\pi}} \int_{U_0} \frac{\partial}{\partial p}\left(\frac{\hat{\psi}(p)}{\frac{\partial \chi(p,q,t)}{\partial p}}\right) e^{\frac{i}{\hbar}\chi(p,q,t)t} dp\end{aligned}$$

so that uniformly on E,

$$\psi(q,t) = O\left(|t|^{-1}\right) \quad \text{as} \quad |t| \to \infty.$$

By repeated integration by parts, we obtain that for every $n \in \mathbb{N}$, uniformly on E,

$$\psi(q,t) = O\left(|t|^{-n}\right)$$

so that $\psi(q,t) = O\left(|t|^{-\infty}\right)$.

To describe the motion of a free quantum particle in unbounded regions, we use the stationary phase method. In its simplest form it is stated as follows.

The Method of Stationary Phase. Let $f, g \in C^\infty(\mathbb{R})$, where f is realvalued and g has compact support, and suppose that f has a single nondegenerate critical point x_0, i.e., $f'(x_0) = 0$ and $f''(x_0) \neq 0$. Then

$$\int_{-\infty}^{\infty} e^{iNf(x)} g(x) dx = \left(\frac{2\pi}{N|f''(x_0)|}\right)^{\frac{1}{2}} e^{iNf(x_0) + \frac{i\pi}{4}\operatorname{sgn} f''(x_0)} g(x_0) + O\left(\frac{1}{N}\right)$$

as $N \to \infty$.

Applying the stationary phase method to the integral representation (2.17) (and setting $N = t$), we find that the critical point of $\chi(p,q,t)$ is $p_0 = \frac{mq}{t}$ with $\chi''(p_0) = -\frac{1}{m} \neq 0$, and

$$\begin{aligned}\psi(q,t) &= \sqrt{\frac{m}{t}} \hat{\psi}\left(\frac{mq}{t}\right) e^{\frac{imq^2}{2\hbar t} - \frac{\pi i}{4}} + O\left(t^{-1}\right) \\ &= \psi_0(q,t) + O\left(t^{-1}\right) \quad \text{as} \quad t \to \infty\end{aligned}$$

Thus as $t \to \infty$, the wave function $\psi(q,t)$ is supported on $\frac{t}{m}U_0$ - a domain where the probability of finding a particle is asymptotically different from zero. At large t the points in this domain move with constant velocities $v = \frac{p}{m}, p \in U_0$. In this sense, the classical relation $p = mv$ remains valid in the quantum picture. Moreover, the asymptotic wave function ψ_0 satisfies

$$\int_{-\infty}^{\infty} |\psi_0(q,t)|^2 dq = \sqrt{\frac{m}{t}} \int_{-\infty}^{\infty} \left|\hat{\psi}\left(\frac{mq}{t}\right)\right|^2 dq = 1$$

and, therefore, describes the asymptotic probability distribution. Similarly, setting $N = -|t|$, we can describe the behavior of the wave function $\psi(q,t)$ as $t \to -\infty$.

Remark. We have $\lim_{|t|\to\infty}\psi(t)=0$ in the weak topology on $\mathscr{H}$. Indeed, for every $\varphi\in\mathscr{H}$ we get by Parseval's identity for the Fourier integrals,

$$(\psi(t),\varphi)=\int_{-\infty}^{\infty}\hat{\psi}(p)\overline{\hat{\varphi}(p)}e^{-\frac{ip^2t}{2m\hbar}}dp$$

and the integral goes to zero as $|t|\to\infty$ by the Riemann-Lebesgue lemma.
A free classical particle with n degrees of freedom is described by the phase space $\mathbb{R}^{2n}$ with coordinates $\boldsymbol{p}=(p_1,...,p_n)$ and $\boldsymbol{q}=(q^1,...,q^n)$, the Poisson bracket (2.3), and the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p},\boldsymbol{q})=\frac{\boldsymbol{p}^2}{2m}=\frac{1}{2m}\left(p_1^2+\cdots+p_n^2\right).$$

The Hamiltonian operator of a free quantum particle with n degrees of freedom is

$$H_0=\frac{\boldsymbol{P}^2}{2m}=\frac{1}{2m}\left(P_1^2+\cdots+P_n^2\right)$$

and in the coordinate representation is

$$H_0=-\frac{\hbar^2}{2m}\Delta$$

where

$$\Delta=\left(\frac{\partial}{\partial\boldsymbol{q}}\right)^2=\left(\frac{\partial}{\partial q^1}\right)^2+\cdots+\left(\frac{\partial}{\partial q^n}\right)^2$$

is the Laplace operator [15] in the Cartesian coordinates on $\mathbb{R}^n$. The Hamiltonian H_0 is a self-adjoint operator on $\mathscr{H}=L^2\left(\mathbb{R}^n,d^n\boldsymbol{q}\right)$ with $D\left(H_0\right)=W^{2,2}\left(\mathbb{R}^n\right)$ - the Sobolev space on $\mathbb{R}^n$. In the momentum representation,

$$H_0=\frac{\boldsymbol{p}^2}{2m}$$

- a multiplication by a function operator on $\mathscr{H}=L^2\left(\mathbb{R}^n,d^n\boldsymbol{p}\right)$.

The operator H_0 is positive with absolutely continuous spectrum $[0,\infty)$ of infinite multiplicity. Namely, let $S^{n-1}=\{n\in\mathbb{R}^n:n^2=1\}$ be the $(n-1)$dimensional unit sphere in $\mathbb{R}^n$, let $d\boldsymbol{n}$ be the measure on S^{n-1} induced by the Lebesgue measure on $\mathbb{R}^n$, and let

$$\mathfrak{h}=\left\{f:S^{n-1}\to\mathbb{C}:\|f\|_{\mathfrak{h}}^2=\int_{S^{n-1}}|f(\boldsymbol{n})|^2dn<\infty\right\}$$

Let $\mathfrak{H}_0^{(n)}=L^2\left(\mathbb{R}_{>0},\mathfrak{h};d\sigma_n\right)$ be the Hilbert space of $\mathfrak{h}$-valued measurable functions [16]Ψ on $\mathbb{R}_{>0}=(0,\infty)$, square-integrable on $\mathbb{R}_{>0}$ with respect to the measure $d\sigma_n(\lambda)=(2m\lambda)^{\frac{n}{2}}\frac{d\lambda}{2\lambda}$,

$$\mathfrak{H}_0^{(n)}=\left\{\Psi:\mathbb{R}_{>0}\to\mathfrak{h},\|\Psi\|^2=\int_0^{\infty}\|\Psi(\lambda)\|_{\mathfrak{h}}^2d\sigma_n(\lambda)<\infty\right\}.$$

When $n=1,\mathfrak{H}_0^{(1)}=\mathfrak{H}_0$ - the corresponding Hilbert space for one degree of freedom. The operator $\mathscr{U}_0:L^2\left(\mathbb{R}^n,d^n\boldsymbol{q}\right)\to\mathfrak{H}_0^{(n)}$,

$$\mathscr{U}_0(\psi)(\lambda)=\Psi(\lambda),\quad\Psi(\lambda)(\boldsymbol{n})=\hat{\psi}(\sqrt{2m\lambda}\boldsymbol{n})$$

[015] It is the negative of the Laplace-Beltrami operator of the standard Euclidean metric on $\mathbb{R}^n$.

is unitary and establishes the isomorphism $L^2(\mathbb{R}^n, d^n\boldsymbol{q}) \simeq \mathfrak{H}_0^{(n)}$. In the momentum representation H_0 is a multiplication by $\frac{1}{2m}\boldsymbol{p}^2$ operator, so that the operator $\mathscr{U}_0 H_0 \mathscr{U}_0^{-1}$ is a multiplication by λ operator in $\mathfrak{H}_0^{(n)}$.

Remark. As in the case $n = 1$, the Hamiltonian operator H_0 has no eigenvectors - the eigenvalue equation

$$H_0\psi = \lambda\psi$$

has no solutions in $L^2(\mathbb{R}^n)$. However, for every $\lambda > 0$ this differential equation has infinitely many linearly independent bounded solutions

$$\psi_{\boldsymbol{n}}(\boldsymbol{q}) = (2\pi\hbar)^{-\frac{n}{2}} e^{\frac{i}{\hbar}\sqrt{2m\lambda}\boldsymbol{n}\boldsymbol{q}}$$

parametrized by the unit sphere S^{n-1}. These solutions do not belong to $L^2(\mathbb{R}^n)$, but in the distributional sense they combine to a Schwartz kernel of the unitary operator $\mathscr{U}_0$, which establishes the isomorphism between $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ and the Hilbert space $\mathfrak{H}_0^{(n)}$, where H_0 acts as a multiplication by λ operator.

As in the case $n = 1$, the Schrodinger equation for free particle,

$$i\hbar\frac{d\psi(t)}{dt} = H_0\psi(t), \quad \psi(0) = \psi$$

is solved by the Fourier transform

$$\psi(\boldsymbol{q}, t) = (2\pi\hbar)^{-n/2} \int_{\mathbb{R}^n} e^{\frac{i}{\hbar}\left(\boldsymbol{p}\boldsymbol{q} - \frac{p^2}{2m}t\right)} \hat{\psi}(\boldsymbol{p}) d^n\boldsymbol{p}$$

For a wave packet, an initial condition ψ such that its Fourier transform $\hat{\psi} = \mathscr{F}_\hbar(\psi)$ is a smooth function supported on a neighborhood U_0 of $\boldsymbol{p}_0 \in \mathbb{R}^n\backslash\{0\}$ such that $0 \notin U_0$ and

$$\int_{\mathbb{R}^n} |\hat{\psi}(\boldsymbol{p})|^2 d^n\boldsymbol{p} = 1$$

the quantum particle leaves every compact subset of $\mathbb{R}^n$ and the motion is infinite. Asymptotically as $|t| \to \infty$, the wave function $\psi(\boldsymbol{q}, t)$ is different from 0 only when $\boldsymbol{q} = \frac{\boldsymbol{p}}{m}t, \boldsymbol{p} \in U_0$.

Problem 2.8. Find the asymptotic wave function for a free quantum particle with n degrees of freedom.

2.4. Examples of quantum systems.

Here we describe quantum systems that correspond to the classical Lagrangian systems introduced in Section 1.3 of Chapter 1. In Hamiltonian formulation, the phase space of these systems, except for the last example, is a symplectic vector space $\mathbb{R}^{2n}$ with canonical coordinates $\boldsymbol{p}, \boldsymbol{q}$ and symplectic form $\omega = d\boldsymbol{p} \wedge d\boldsymbol{q}$.

Example 2.1 (Newtonian particle). According to Section 1.7 in Chapter 1, a classical particle in $\mathbb{R}^n$ moving in a potential field $V(\boldsymbol{q})$ is described by the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{q}) = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{q})$$

Assume that the Hamiltonian operator for the quantum system is given by

$$H = \frac{\boldsymbol{P}^2}{2m} + V,$$

[016] That is, for every $f \in \mathfrak{h}$ the function (f, Ψ) is measurable on $\mathbb{R}_{>0}$.

with some operator V, so that coordinate and momenta operators satisfy Heisenberg equations of motion

$$\dot{\boldsymbol{P}} = \{H, \boldsymbol{P}\}_\hbar, \dot{\boldsymbol{Q}} = \{H, \boldsymbol{Q}\}_\hbar \tag{2.19}$$

To determine V, we require that the classical relation $\dot{\boldsymbol{q}} = \frac{\boldsymbol{p}}{m}$ between the velocity and the momentum of a particle is preserved under the quantization, i.e.,

$$\dot{\boldsymbol{Q}} = \frac{\boldsymbol{P}}{m}$$

Since $\{\boldsymbol{P}^2, \boldsymbol{Q}\}_\hbar = 2\boldsymbol{P}$, it follows from (2.19) that this condition is equivalent to

$$[V, Q_k] = 0, \quad k = 1, ..., n$$

It follows from Section 2.2 that V is a function of commuting operators $Q_1, ..., Q_n$, and the natural choice [17] is $V = V(\boldsymbol{Q})$. Thus the Hamiltonian operator of a Newtonian particle is

$$H = \frac{\boldsymbol{P}^2}{2m} + V(\boldsymbol{Q})$$

in agreement with $H = H_{\mathrm{c}}(\boldsymbol{P}, \boldsymbol{Q})$[18]. In coordinate representation the Hamiltonian is the Schrodinger operator

$$H = -\frac{\hbar^2}{2m}\Delta + V(\boldsymbol{q}) \tag{2.20}$$

with the real-valued potential $V(\boldsymbol{q})$.

Remark. The sum of two unbounded, self-adjoint operators is not necessarily self-adjoint, and one needs to describe admissible potentials $V(\boldsymbol{q})$ for which H is a self-adjoint operator on $L^2(\mathbb{R}^n, d^n\boldsymbol{q})$. If the potential $V(\boldsymbol{q})$ is a real-valued, locally integrable function on $\mathbb{R}^n$, then the differential operator (2.20) defines a symmetric operator H with the domain $C_0^2(\mathbb{R}^n)$ - twice continuously differentiable functions on $\mathbb{R}^n$ with compact support. Potentials for which the symmetric operator H has no self-adjoint extensions are obviously non-physical. It may also happen that H has several self-adjoint extensions [19]. These extensions are specified by some boundary conditions at infinity and there are no physical principles distinguishing between them. The only physical case is when the symmetric operator H admits a unique self-adjoint extension, that is, when H is essentially self-adjoint. In Chapter 3 we present necessary conditions for the essential self-adjointness. Here we only mention the von Neumann criterion that if A is a closed operator and $\overline{D(A)} = \mathscr{H}$, then $H = A^*A$ is a positive self-adjoint operator.

Example 2.2 (Interacting quantum particles). In Lagrangian formalism, a closed classical system of N interacting particles on $\mathbb{R}^3$ was described in Example 1.2 in Section 1.3 of Chapter 1. In Hamiltonian formalism, it is described by the canonical coordinates $r = (\boldsymbol{r}_1, ..., \boldsymbol{r}_N)$, the canonical momenta $\boldsymbol{p} = (\boldsymbol{p}_1, ..., \boldsymbol{p}_N), \boldsymbol{r}_a, \boldsymbol{p}_a \in \mathbb{R}^3$, and by the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{r}) = \sum_{a=1}^{N} \frac{\boldsymbol{p}_a^2}{2m_a} + V(\boldsymbol{r}) \tag{2.21}$$

where m_a is the mass of the a-th particle, $a = 1, ..., N$ (see Section 1.7 in Chapter 1). The corresponding Hamiltonian operator H in the coordinate representation has the form

$$H = -\sum_{a=1}^{N} \frac{\hbar^2}{2m_a}\Delta_a + V(\boldsymbol{r}) \tag{2.22}$$

[017] Confirmed by the agreement of the theory with the experiments.

In particular, when

$$V(\boldsymbol{r}) = \sum_{1\le a<b\le N} V\left(\boldsymbol{r}_a - \boldsymbol{r}_b\right),$$

the Schrodinger operator (2.22) describes the N-body problem in quantum mechanics. The fundamental quantum system is the complex atom, formed by a nucleus of charge Ne and mass M, and by N electrons of charge $-e$ and mass m. Denoting by $\boldsymbol{R} \in \mathbb{R}^3$ the position of the nucleus, and by $\boldsymbol{r}_1, ..., \boldsymbol{r}_N$ the positions of the electrons and assuming that the interaction is given by the Coulomb attraction, we get for the Hamiltonian function (2.21)

$$H_{\mathrm{c}}(\boldsymbol{P}, \boldsymbol{p}, \boldsymbol{R}, \boldsymbol{r}) = \frac{\boldsymbol{P}^2}{2M} + \sum_{a=1}^{N} \frac{\boldsymbol{p}_a^2}{2m} - \sum_{a=1}^{N} \frac{Ne^2}{|\boldsymbol{R} - \boldsymbol{r}_a|} + \sum_{1\le a<b\le N} \frac{e^2}{|\boldsymbol{r}_a - \boldsymbol{r}_b|},$$

where $\boldsymbol{P}$ is the canonical momentum of the nucleus. The corresponding Schrodinger operator H in the coordinate representation has the form [20]

$$H = -\frac{\hbar^2}{2M}\Delta - \sum_{a=1}^{N} \frac{\hbar^2}{2m}\Delta_a - \sum_{a=1}^{N} \frac{Ne^2}{|\boldsymbol{R} - \boldsymbol{r}_a|} + \sum_{1\le a<b\le N} \frac{e^2}{|\boldsymbol{r}_a - \boldsymbol{r}_b|}$$

In the simplest case of the hydrogen atom, when $N = 1$ and the nucleus consists of a single proton [21], the Hamiltonian is

$$H = -\frac{\hbar^2}{2M}\Delta_p - \frac{\hbar^2}{2m}\Delta_e - \frac{e^2}{|\boldsymbol{r}_p - \boldsymbol{r}_e|}$$

where $\boldsymbol{r}_p$ is the position of the proton and $\boldsymbol{r}_e$ is the position of the electron. As the first approximation, the proton can be considered as infinitely heavy, so that the hydrogen atom is described by an electron in an attractive Coulomb field $-e^2/|\boldsymbol{r}|$, where now $\boldsymbol{r} = \boldsymbol{r}_e - \boldsymbol{r}_p$. The corresponding Hamiltonian operator takes the form

$$H = -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{|\boldsymbol{r}|} \tag{2.23}$$

We will solve the Schrodinger equation with this Hamiltonian H and determine its energy levels in Section 5.1 of Chapter 3.

Example 2.3 (Charged particle in an electromagnetic field). A classical particle of charge e and mass m moving in the time-independent electromagnetic field with scalar and vector potentials $\varphi(\boldsymbol{r})$ and $\boldsymbol{A}(\boldsymbol{r}), \boldsymbol{r} \in \mathbb{R}^3$, is described by the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{r}) = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 + e\varphi(\boldsymbol{r})$$

(see Problem 1.27 in Section 1.7 of Chapter 1). The corresponding classical velocity vector $\boldsymbol{v} = \{H_{\mathrm{c}}, \boldsymbol{r}\}$ is given by

$$v = p - \frac{e}{c}A$$

[018] In the special case $H_c(\boldsymbol{p}, \boldsymbol{q}) = f(\boldsymbol{p}) + g(\boldsymbol{q})$ the problem of the ordering of non-commuting operators $\boldsymbol{P}$ and $\boldsymbol{Q}$ does not arise.

[19] This is the case when the defect indices of H are equal and are non-zero.

[020] Ignoring the fact that electron has spin, see Chapter 4.

[21] In the case of hydrogen-1 or protium; it includes one or more neutrons for deuterium, tritium, and other isotopes.

and its components $\boldsymbol{v} = (v_1, v_2, v_3)$ have non-vanishing Poisson brackets:

$$\{v_1, v_2\} = -\frac{e}{m^2c}B_3, \quad \{v_2, v_3\} = -\frac{e}{m^2c}B_1, \quad \{v_3, v_1\} = -\frac{e}{m^2c}B_2,$$

where $\boldsymbol{B} = (B_1, B_2, B_3)$ are components of the magnetic field $\boldsymbol{B} = \operatorname{curl} \boldsymbol{A}$.
The Hamiltonian operator of a quantum particle is

$$H = \frac{1}{2m}\left(\boldsymbol{P} - \frac{e}{c}\boldsymbol{A}\right)^2 + e\varphi(\boldsymbol{r}) \tag{2.24}$$

- the Schrodinger operator of a charged particle in an electromagnetic field. The corresponding quantum velocity vector $\boldsymbol{V} = \{H, \boldsymbol{Q}\}_\hbar$ is given by the same formula as in the classical case,

$$V = P - \frac{e}{c}A,$$

and its components $\boldsymbol{V} = (V_1, V_2, V_3)$ have non-vanishing quantum brackets:

$$\{V_1, V_2\}_\hbar = -\frac{e}{m^2c}B_3, \qquad \{V_2, V_3\}_\hbar = -\frac{e}{m^2c}B_1, \qquad \{V_3, V_1\}_\hbar = -\frac{e}{m^2c}B_2$$

Thus in the presence of a magnetic field the three components of a quantum velocity operator no longer commute and cannot be measured simultaneously.

Example 2.4 (Free quantum particle on a Riemannian manifold). The phase space of a classical particle of mass $m = 1$ moving on a Riemannian manifold (M, g) is the cotangent bundle T^*M, and the corresponding Hamiltonian function is given by

$$H_c(\boldsymbol{p}, \boldsymbol{x}) = \frac{1}{2}g^{\mu\nu}(\boldsymbol{x})p_\mu p_\nu,$$

where $g^{\mu\nu}(\boldsymbol{x})$ is the inverse of the metric tensor $g_{\mu\nu}(\boldsymbol{x})$, and

$$(\boldsymbol{p}, \boldsymbol{x}) = \left(p_1, ..., p_n, x^1, ..., x^n\right)$$

are standard coordinates on T^*M (see Section 1.7 of Chapter 1). The Hilbert space of the quantum system is $\mathscr{H} = L^2(M, d\mu)$, where $d\mu = \sqrt{g(\boldsymbol{x})}d^n\boldsymbol{x}$, $g(\boldsymbol{x}) = \det\left(g_{\mu\nu}(\boldsymbol{x})\right)$, is the measure associated with the density of the Riemannian metric (Riemannian volume form if M is oriented). When canonical coordinates $(\boldsymbol{p}, \boldsymbol{x})$ are only locally defined on T^*M, it is not possible to construct corresponding operators $\boldsymbol{P}$ and $\boldsymbol{Q}$. Still, one can always define the Hamiltonian operator by

$$H = \frac{\hbar^2}{2}\Delta_g, \quad \text{where} \quad \Delta_g = -\frac{1}{\sqrt{g(\boldsymbol{x})}}\frac{\partial}{\partial x^\mu}\left(\sqrt{g(\boldsymbol{x})}g^{\mu\nu}\frac{\partial}{\partial x^\nu}\right) \tag{2.25}$$

is the Laplace-Beltrami operator of the Riemannian metric g on M. Note that in this case there is a non-trivial problem of the ordering of noncommuting operators in the quantization of $H_c(\boldsymbol{p}, \boldsymbol{x})$, which arises if in a
coordinate chart on M one replaces canonical coordinates $\boldsymbol{p}$ and $\boldsymbol{x}$ by $\boldsymbol{P}$ and $\boldsymbol{Q}$. The formula

$$\Delta_g = -g^{\mu\nu}(\boldsymbol{x})\frac{\partial^2}{\partial x^\mu \partial x^\nu} + g^{\mu\sigma}(\boldsymbol{x})\Gamma^\nu_{\mu\sigma}(\boldsymbol{x})\frac{\partial}{\partial x^\nu}$$

shows that local expressions defined by

$$H_c(\boldsymbol{P}, \boldsymbol{Q}) = \frac{1}{2}\left(g^{\mu\nu}(\boldsymbol{Q})P_\mu P_\nu + i\hbar g^{\mu\sigma}(\boldsymbol{Q})\Gamma^\nu_{\mu\sigma}(\boldsymbol{Q})P_\nu\right) \tag{2.26}$$

combine to a well-defined self-adjoint operator H on $\mathscr{H}$ given by (2.25). Thus even when $M = \mathbb{R}^n$ and canonical coordinates $(\boldsymbol{p}, \boldsymbol{x})$ are globally defined on $T^*\mathbb{R}^n$, the correct formula for $H_c(\boldsymbol{P}, \boldsymbol{Q})$ - the one which extends to general Riemannian manifolds - is given by (2.26), where the second term represents the "quantum correction" to the naive expression $g^{\mu\nu}(\boldsymbol{Q})P_\mu P_\nu$.

2.5. Old quantum mechanics.

The formulation of quantum mechanics presented here goes back to 1925-1927, and is due to Heisenberg, Schrodinger, Born, Jordan, and Dirac. It replaced the old quantum theory, proposed in 1913 by Bohr, which was based on Rutherford's planetary model of the atom. In the old theory, the energy levels of a one-dimensional quantum system correspond to the closed orbits of the associated classical Hamiltonian system which satisfy the Bohr-Wilson-Sommerfeld quantization rule (BWS rule)

$$\oint p dq = 2\pi\hbar \left(n + \frac{1}{2}\right)$$

where n is a non-negative integer, and integration goes over the closed orbit in the phase space $\mathbb{R}^2$. Bohr-Wilson-Sommerfeld quantization rules also apply to completely integrable Hamiltonian systems with several degrees of freedom (see Section 2.6 of Chapter 1). Namely, let $F_1 = H_c, ..., F_N$ be N independent integrals of motion in involution. The BWS quantization rules are

$$\oint_\gamma \boldsymbol{p} d\boldsymbol{q} = 2\pi\hbar \left(n_\gamma + \frac{1}{4} \operatorname{ind} \gamma\right),$$

where integration goes over all 1-cycles γ in the Lagrangian submanifold $\Lambda = \left\{(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{R}^{2N} : H_c(\boldsymbol{p}, \boldsymbol{q}) = E, F_2(\boldsymbol{p}, \boldsymbol{q}) = E_2, ..., F_N(\boldsymbol{p}, \boldsymbol{q}) = E_N\right\}$, and $\operatorname{ind} \gamma \in \mathbb{Z}$ is the so-called Maslov index of a cycle γ in Λ. In the onedimensional case the closed orbit is topologically a circle and its Maslov index is 2 . It will be shown in Section 6.3 of Chapter 3 that, in general, Bohr-Wilson-Sommerfeld quantization rules only give asymptotics of the energy levels as $\hbar \to 0$. However, for integrable systems with extra symmetry, such as the harmonic oscillator and the Kepler problem, the BWS quantization rules determine the energy levels exactly. We will show this in the next section for the harmonic oscillator, and in Section 5.1 of Chapter 3 - for the Kepler problem.

2.6. Harmonic oscillator.

The simplest classical system with one degree of freedom, besides the free particle, is the harmonic oscillator. It is described by the phase space $\mathbb{R}^2$ with the canonical coordinates p, q, and the Hamiltonian function

$$H_c(p, q) = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2} \tag{2.27}$$

(see Sections 1.5 and 1.7 in Chapter 1). Hamilton's equations

$$\dot{p} = \{H_c, p\} = -m\omega^2 q, \quad \dot{q} = \{H_c, q\} = \frac{p}{m}$$

with the initial conditions p_0, q_0 are readily solved,

$$p(t) = p_0 \cos \omega t - m\omega q_0 \sin \omega t \tag{2.28}$$

$$q(t) = q_0 \cos \omega t + \frac{1}{m\omega} p_0 \sin \omega t \tag{2.29}$$

and describe the harmonic motion. As in Section 2.6 of Chapter 1, it is convenient to introduce complex coordinates on the phase space on $\mathbb{R}^2 \simeq \mathbb{C}$,

$$z = \frac{1}{\sqrt{2\omega}}(\omega q + ip), \quad \bar{z} = \frac{1}{\sqrt{2\omega}}(\omega q - ip). \tag{2.30}$$

We have

$$\{z, \bar{z}\} = \frac{i}{m}, \quad H_{\mathrm{c}}(z, \bar{z}) = m\omega|z|^2 \tag{2.31}$$

so that Hamilton's equations decouple,

$$\dot{z} = \{H_{\mathrm{c}}, z\} = -i\omega z, \quad \dot{\bar{z}} = \{H_{\mathrm{c}}, \bar{z}\} = i\omega\bar{z}$$

and are trivially solved,

$$z(t) = e^{-i\omega t} z_0, \quad \bar{z} = e^{i\omega t}\bar{z}_0. \tag{2.32}$$

Here

$$z_0 = \frac{1}{\sqrt{2\omega}}\left(\omega q_0 + ip_0\right), \quad \bar{z}_0 = \frac{1}{\sqrt{2\omega}}\left(\omega q_0 - ip_0\right).$$

For the quantum system, the corresponding Hamiltonian operator is

$$H = \frac{P^2}{2m} + \frac{m\omega^2 Q^2}{2},$$

and in the coordinate representation $\mathscr{H} = L^2(\mathbb{R}, dq)$ it is a Schrodinger operator with a quadratic potential,

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{m\omega^2 q^2}{2}.$$

The quantum harmonic oscillator is the simplest non-trivial quantum system, besides the free particle, whose Schrodinger equation can be solved explicitly. It appears in all problems involving quantized oscillations, namely in molecular and crystalline vibrations. The exact solution of the harmonic
oscillator, described below, has remarkable [22] algebraic and analytic properties.

Temporarily set $m = 1$ and consider the operators

$$a = \frac{1}{\sqrt{2\omega\hbar}}(\omega Q + iP), \quad a^* = \frac{1}{\sqrt{2\omega\hbar}}(\omega Q - iP) \tag{2.33}$$

which are quantum analogs of complex coordinates (2.30). The operators a and a^* are defined on $W^{1,2}(\mathbb{R}) \cap \widehat{W}^{1,2}(\mathbb{R})$, where $\widehat{W}^{1,2}(\mathbb{R}) = \mathscr{F}\left(W^{1,2}(\mathbb{R})\right)$, and it is easy to show that a^* is the adjoint operator to a and $a^{**} = a$, so that a is a closed operator. From the Heisenberg commutation relation (2.2) we get the canonical commutation relation

$$[a, a^*] = I \tag{2.34}$$

on $W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$. Indeed,

$$aa^* = \frac{P^2 + \omega^2 Q^2}{2\omega\hbar} + \frac{i\omega}{2\omega\hbar}[P, Q] = \frac{P^2 + \omega^2 Q^2}{2\omega\hbar} + \frac{1}{2}I,$$

and

$$a^* a = \frac{P^2 + \omega^2 Q^2}{2\omega\hbar} - \frac{i\omega}{2\omega\hbar}[P, Q] = \frac{P^2 + \omega^2 Q^2}{2\omega\hbar} - \frac{1}{2}I,$$

so that (2.34) holds on $W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$, where $\widehat{W}^{2,2}(\mathbb{R}) = \mathscr{F}\left(W^{2,2}(\mathbb{R})\right)$, and

$$H = \omega\hbar\left(a^*a + \frac{1}{2}I\right) = \omega\hbar\left(aa^* - \frac{1}{2}I\right).$$

In particular, it follows from the von Neumann criterion that the Hamiltonian operator H is self-adjoint.

The operators a, a^* and $N = a^*a$ satisfy the commutation relations

$$[N, a] = -a, \quad [N, a^*] = a^*, \quad [a, a^*] = I. \tag{2.35}$$

These commutation relations correspond to the irreducible unitary representation of a four-dimensional solvable Lie algebra $\tilde{\mathfrak{h}}$ associated with the Heisenberg algebra $\mathfrak{h} = \mathfrak{h}_1$, introduced in Section 2.1. Namely, $\mathfrak{h}$ is a Lie algebra with the generators e, f, h, and c, where e, f, c satisfy the relations of the Heisenberg algebra $\mathfrak{h}$, and

$$[h, e] = -f, \quad [h, f] = \omega^2 e, \quad [h, c] = 0.$$

The irreducible integrable representation ρ of the Heisenberg algebra $\mathfrak{h}$ (see (2.9) in Section 2.1) extends to a unitary representation of the Lie algebra
$\tilde{\mathfrak{h}}$ by setting

$$\rho(h) = -i\omega N = \frac{P^2 + \omega^2 Q^2}{2i\hbar} + \frac{i\omega}{2}I.$$

Remark. In invariant terms, the Lie algebra $\tilde{\mathfrak{h}}$ is a one-dimensional right extension of the Heisenberg algebra $\mathfrak{h}$,

$$0 \to \mathfrak{h} \to \tilde{\mathfrak{h}} \to \mathbb{R} \to 0$$

It is defined by the $\mathfrak{h}$-valued Lie algebra 1-cocycle $r \in Z^1(\mathfrak{h}, \mathfrak{h})$ - a derivation of $\mathfrak{h}$, given on generators by

$$r(e) = f, \quad r(f) = -\omega^2 e, \quad r(c) = 0$$

Explicitly, if $h \in \tilde{\mathfrak{h}}$ is such that $\bar{h} = 1 \in \mathbb{R}$ under the projection $\tilde{\mathfrak{h}} \to \mathbb{R}$, then identifying elements in $\mathfrak{h}$ with their images under the embedding $\mathfrak{h} \hookrightarrow \tilde{\mathfrak{h}}$, we have

$$[x + \alpha h, y + \beta h] = [x, y] - \alpha r(y) + \beta r(y), \quad x, y \in \mathfrak{h}.$$

It is due to this Lie-algebraic structure of commutation relations (2.35) that Heisenberg equations of motion for the harmonic oscillator can be solved exactly. Namely, we have

$$\dot{a} = \{H, a\}_\hbar = -i\omega a, \quad \dot{a}^* = \{H, a^*\}_\hbar = i\omega a^*,$$

so that

$$a(t) = e^{-i\omega t}a_0, \quad a^*(t) = e^{i\omega t}a_0^*.$$

Comparing with (2.32) we see that solutions of classical and quantum equations of motion for the harmonic oscillator have the same form!

Next, using commutation relations (2.35) and positivity of the operator N, we will solve the eigenvalue problem for the Hamiltonian H of the harmonic oscillator explicitly by finding its energy levels and corresponding eigenvectors. We will prove that the eigenvectors form

[022] The algebraic structure of the exact solution of the harmonic oscillator plays a fundamental role in quantum electrodynamics and in quantum field theory in general.

a complete system of vectors in $\mathscr{H}$, so that the spectrum of the Hamiltonian H is the point spectrum. This is a quantum mechanical analog of the fact that classical motion of the harmonic oscillator is always finite.

The algebraic part of the exact solution is the following fundamental result.

Proposition 2.2. Suppose that there exists a non-zero $\psi \in D(a^n) \cap D((a^*)^n)$, $n = 1, 2, ...$, such that

$$H\psi = \lambda\psi.$$

Then the following statements hold.

(i) There exists $\psi_0 \in \mathscr{H}$, $\|\psi_0\| = 1$, such that

$$H\psi_0 = \frac{1}{2}\hbar\omega\psi_0.$$

(ii) The vectors

$$\psi_n = \frac{(a^*)^n}{\sqrt{n!}}\psi_0 \in \mathscr{H}, \quad n = 0, 1, 2, ...,$$

are orthonormal eigenvectors for H with the eigenvalues $\hbar\omega\left(n + \frac{1}{2}\right)$,

$$H\psi_n = \hbar\omega\left(n + \frac{1}{2}\right)\psi_n.$$

(iii) Restriction of the operator H to the Hilbert space $\mathscr{H}_0 - a$ closed subspace of $\mathscr{H}$, spanned by the orthonormal set $\{\psi_n\}_{n=0}^{\infty}$ - is essentially self-adjoint.

Proof. Rewriting commutation relations (2.35) as

$$Na = a(N - I) \quad \text{and} \quad Na^* = a^*(N + I),$$

and putting $\lambda = \hbar\omega\left(\mu + \frac{1}{2}\right)$, we get for all $n \geq 0$,

$$Na^n\psi = (\mu - n)a^n\psi \quad \text{and} \quad N(a^*)^n\psi = (\mu + n)(a^*)^n\psi. \tag{2.36}$$

Since $N \geq 0$ on $D(N)$, it follows from the first equation in (2.36) that there exists $n_0 \geq 0$ such that $a^{n_0}\psi \neq 0$ but $a^{n_0+1}\psi = 0$. Setting $\psi_0 = \frac{a^{n_0}\psi}{\|a^{n_0}\psi\|} \in \mathscr{H}$ we get

$$a\psi_0 = 0 \quad \text{and} \quad N\psi_0 = 0 \tag{2.37}$$

Since $H = \hbar\omega\left(N + \frac{1}{2}I\right)$, this proves part (i). To prove part (ii), we use commutation relations

$$[a, (a^*)^n] = n(a^*)^{n-1}, \tag{2.38}$$

which follow from (2.34) and the Leibniz rule. Using (2.37)-(2.38), we get

$$a^*\psi_n = \sqrt{n+1}\psi_{n+1}, \quad a\psi_n = \sqrt{n}\psi_{n-1}, \tag{2.39}$$

so that

$$\|\psi_n\|^2 = \frac{1}{\sqrt{n}}(a^*\psi_{n-1}, \psi_n) = \frac{1}{\sqrt{n}}(\psi_{n-1}, a\psi_n) = \|\psi_{n-1}\|^2 = \cdots = \|\psi_0\|^2 = 1.$$

From the second equation in (2.36) it follows that $N\psi_n = n\psi_n$, so ψ_n are normalized eigenvectors of H with the eigenvalues $\hbar\omega\left(n + \frac{1}{2}\right)$. The eigenvectors ψ_n are orthogonal since the corresponding eigenvalues are distinct and the operator H is symmetric. Finally, part (iii)

immediately follows from the fact that, according to part (ii), the subspaces $\mathrm{Im}(H \pm iI)|_{\mathscr{H}_0}$ are dense in $\mathscr{H}_0$, which is the criterion of essential self-adjointness.

Remark. Since the coordinate representation of the Heisenberg commutation relations is irreducible, it is tempting to conclude, using Proposition 2.2, that $\mathscr{H}_0 = \mathscr{H}$. Namely, it follows from the construction that the linear span of vectors ψ_n - a dense subspace of $\mathscr{H}_0$ - is invariant for the operators P and Q. However, this does not immediately imply that the projection operator Π_0 onto the subspace $\mathscr{H}_0$ commutes with self-adjoint operators P and Q in the sense of the definition in Section 1.1.

Using the coordinate representation, we can immediately show the existence of the vector ψ_0 in Proposition 2.2, and prove that $\mathscr{H}_0 = \mathscr{H}$. Indeed, equation $a\psi_0 = 0$ becomes a first order linear differential equation

$$\left(\hbar\frac{d}{dq} + \omega q\right)\psi_0 = 0$$

so that

$$\psi_0(q) = \sqrt[4]{\frac{\omega}{\pi\hbar}}e^{-\frac{\omega}{2\pi}q^2},$$

and

$$\|\psi_0\|^2 = \sqrt{\frac{\omega}{\pi\hbar}}\int_{-\infty}^{\infty} e^{-\frac{\omega}{\hbar}q^2}dq = 1$$

The vector ψ_0 is called the ground state for the harmonic oscillator. Correspondingly, the eigenfunctions

$$\psi_n(q) = \frac{1}{\sqrt{n!}}\left(\frac{1}{\sqrt{2\omega\hbar}}\left(\omega q - \hbar\frac{d}{dq}\right)\right)^n\psi_0$$

are of the form $P_n(q)e^{-\frac{\omega}{2\hbar}q^2}$, where $P_n(q)$ are polynomials of degree n. The following result guarantees that the functions $\{\psi_n\}_{n=0}^{\infty}$ form an orthonormal basis in $L^2(\mathbb{R}, dq)$.

Lemma 2.3. The functions $q^n e^{-q^2}, n = 0, 1, 2, ...$, are complete in $L^2(\mathbb{R}, dq)$.

Proof. Let $f \in L^2(\mathbb{R}, dq)$ is such that

$$\int_{-\infty}^{\infty} f(q)q^n e^{-q^2}dq = 0, \quad n = 0, 1, 2, ...$$

The integral

$$F(z) = \int_{-\infty}^{\infty} f(q)e^{iqz-q^2}dq$$

is absolutely convergent for all $z \in \mathbb{C}$ and, therefore, defines an entire function. We have

$$F^{(n)}(0) = i^n\int_{-\infty}^{\infty} f(q)q^n e^{-q^2}dq = 0, \quad n = 0, 1, 2, ...$$

so that $F(z) = 0$ for all $z \in \mathbb{C}$. This implies the function $g(q) = f(q)e^{-q^2} \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ satisfies $\mathscr{F}(g) = 0$, where $\mathscr{F}$ is the "ordinary" ($\hbar = 1$) Fourier transform. Thus we conclude that $g = 0$.

The polynomials P_n are expressed through classical Hermite-Tchebyscheff polynomials H_n, defined by

$$H_n(q) = (-1)^n e^{q^2}\frac{d^n}{dq^n}e^{-q^2}, \quad n = 0, 1, 2, ...$$

Namely, using the identity

$$e^{\frac{q^2}{2}}\frac{d^n}{dq^n}e^{-q^2} = -\left(q-\frac{d}{dq}\right)\left[e^{\frac{q^2}{2}}\frac{d^{n-1}}{dq^{n-1}}e^{-q^2}\right]$$
$$= \cdots = (-1)^n\left(q-\frac{d}{dq}\right)^n e^{-\frac{q^2}{2}}$$

we obtain

$$\psi_n(q) = \sqrt[4]{\frac{\omega}{\pi\hbar}}\frac{1}{\sqrt{2^n n!}}e^{-\frac{\omega}{2\hbar}q^2}H_n\left(\sqrt{\frac{\omega}{\hbar}}q\right).$$

We summarize the obtained results as follows.

Theorem 2.1. The Hamiltonian

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{m\omega^2 q^2}{2}$$

of the quantum harmonic oscillator with one degree of freedom is a selfadjoint operator on $\mathscr{H} = L^2(\mathbb{R}, dq)$ with the domain $D(H) = W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$. The operator H has pure point spectrum

$$H\psi_n = \lambda_n\psi_n, \quad n = 0, 1, 2, ...$$

with the eigenvalues $\lambda_n = \hbar\omega\left(n+\frac{1}{2}\right)$. Corresponding eigenfunctions ψ_n form an orthonormal basis for $\mathscr{H}$ and are given by

$$\psi_n(q) = \sqrt[4]{\frac{m\omega}{\pi\hbar}}\frac{1}{\sqrt{2^n n!}}e^{-\frac{m\omega}{2\hbar}q^2}H_n\left(\sqrt{\frac{m\omega}{\hbar}}q\right) \tag{2.40}$$

where $H_n(q)$ are classical Hermite-Tchebyscheff polynomials.

Proof. Consider the operator H defined on the Schwartz space $\mathscr{S}(\mathbb{R})$ of rapidly decreasing functions. Since the operator H is symmetric and has a complete system of eigenvectors in $\mathscr{S}(\mathbb{R})$, the subspaces $\mathrm{Im}(H \pm iI)$ are dense in $\mathscr{H}$, so that H is essentially self-adjoint. The proof that its self-adjoint closure (which we continue to denote by H) has the domain $W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$ is left to the reader.

Remark. The energy levels of the harmonic oscillator can be also obtained from the Bohr-Wilson-Sommerfeld quantization rule. Indeed, the corresponding classical orbit with the energy E is an ellipse in the phase plane
given by the equations $q(t) = A\cos(\omega t + \alpha), p(t) = -m\omega A\sin(\omega t + \alpha)$, where $E = \frac{1}{2}m\omega^2 A^2$ (see Section 1.5 in Chapter 1). Thus

$$\oint pdq = \iint dp \wedge dq = \pi m\omega A^2 = \frac{2\pi}{\omega}E,$$

and the BWS quantization rule gives the energy levels $E_n = \hbar\omega\left(n+\frac{1}{2}\right)$.

Remark. Since the energy levels of the Hamiltonian H are equidistant by $\hbar\omega$, the quantum harmonic oscillator describes the system of identical "quanta" with the energy $\hbar\omega$. The ground state $|0\rangle = \psi_0$, in Dirac's notation, is the vacuum state with no quanta present and with the vacuum energy $\frac{1}{2}\hbar\omega$, and the states $|n\rangle = \psi_n$ consist of n quanta with the energy $\hbar\omega\left(n+\frac{1}{2}\right)$. According to (2.39), the operator a^* adds one quantum to the state $|n\rangle$ and is called a creation operator, and the operator a destroys one quantum in the state $|n\rangle$ and is called an annihilation operator.

An example of the harmonic oscillator illustrates the dramatic difference between the motion in quantum mechanics and in classical mechanics. The classical motion in the potential field

$V(q) = \frac{1}{2}m\omega^2 q^2$ is finite: a particle with energy E moves in the region $|\omega q| \leq \sqrt{\frac{2E}{m}}$, whereas there is always a non-zero probability of finding a quantum particle outside the classical region. Thus for the ground state energy $E = \frac{1}{2}\hbar\omega$ this probability is

$$\int_{|q|\geq\sqrt{\frac{\hbar}{m\omega}}} |\psi_0(q)|^2 \, dq = \frac{2}{\sqrt{\pi}} \int_1^\infty e^{-x^2} dx \simeq 0.1572992070.$$

The classical harmonic oscillator with n degrees of freedom is described by the phase space $\mathbb{R}^{2n}$ with the canonical coordinates $\boldsymbol{p}, \boldsymbol{q}$, and the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{q}) = \frac{\boldsymbol{p}^2}{2m} + \sum_{j=1}^n \frac{m\omega_j^2 q_j^2}{2},$$

where $\omega_1, ..., \omega_n > 0$ (see Sections 1.3 and 1.7 in Chapter 1).
The corresponding Hamiltonian operator is

$$H = \frac{\boldsymbol{P}^2}{2m} + \sum_{j=1}^n \frac{m\omega_j^2 Q_j^2}{2}$$

and in the coordinate representation $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ is a Schrodinger operator with quadratic potential,

$$H = -\frac{\hbar^2}{2m}\Delta + \sum_{j=1}^n \frac{m\omega_j^2 q_j^2}{2}.$$

The Hamiltonian H is a self-adjoint operator with $D(H) = W^{2,2}(\mathbb{R}^n) \cap \widehat{W}^{2,2}(\mathbb{R}^n)$ and a pure point spectrum. The corresponding eigenfunctions

$$\psi_{\boldsymbol{k}}(\boldsymbol{q}) = \psi_{k_1}(q_1) ... \psi_{k_n}(q_n)$$

where $\boldsymbol{k} = (k_1, ..., k_n)$ and $\psi_{k_j}(q_j)$ are eigenfunctions (2.40) with $\omega = \omega_j$, form an orthonormal basis for $L^2(\mathbb{R}^n, d^n\boldsymbol{q})$. The corresponding energy levels are given by

$$\lambda_{\boldsymbol{k}} = \hbar\omega_1\left(k_1 + \frac{1}{2}\right) + \cdots + \hbar\omega_n\left(k_n + \frac{1}{2}\right)$$

The spectrum of H is simple if and only if $\hbar\omega_1, ..., \hbar\omega_n$ are linearly independent over $\mathbb{Z}$. The highest degeneracy case is $\omega_1 = \cdots = \omega_n = \omega$, when the multiplicity of the eigenvalue

$$\lambda_k = \hbar\omega \sum_{j=1}^n \left(k_j + \frac{1}{2}\right)$$

is the partition function $p_n(|\boldsymbol{k}|)$ - the number of representations of the integer $|\boldsymbol{k}| = k_1 + \cdots + k_n$ as a sum of n non-negative integers. Setting $m = 1$ and introducing the operators [23]

$$a_j = \frac{1}{\sqrt{2\omega\hbar}}(\omega Q_j + iP_j), \quad a_j^* = \frac{1}{\sqrt{2\omega\hbar}}(\omega Q_j - iP_j), \quad j = 1, ..., n \tag{2.41}$$

we get canonical commutation relations for creation and annihilation operators for n degrees of freedom,

$$[a_j, a_l] = 0, \quad \left[a_j^*, a_l^*\right] = 0, \quad [a_j, a_l^*] = \delta_{jl}I, \quad j, l = 1, ..., n, \tag{2.42}$$

which generalize relation (2.34) for the one degree of freedom. The operators a_j, a_j^* and $N_j = a_j^* a_j, j = 1, ..., n$, satisfy commutation relations

$$[N_j, a_l] = -\delta_{jl} a_l, \quad [N_j, a_l^*] = \delta_{jl} a_l^*, \quad j, l = 1, ..., n \tag{2.43}$$

In particular, the operator

$$N = \sum_{j=1}^{n} N_j = \sum_{j=1}^{n} a_j^* a_j$$

satisfies

$$[N, a_j] = -a_j, \quad \left[N, a_j^*\right] = a_j^*, \quad j = 1, ..., n,$$

and $H = \hbar\omega\left(N + \frac{n}{2} I\right)$.

Commutation relations (2.42) and (2.43) correspond to the irreducible unitary representation of the solvable Lie algebra $\tilde{\mathfrak{h}}_n$ with $3n+1$ generators e_j, f_j, h_j, and c, where e_j, f_j, c satisfy the relations in the Heisenberg algebra $\mathfrak{h}_n$, and

$$[h_j, e_l] = -\delta_{jl} f_l, \quad [h_j, f_l] = \delta_{jl}\omega_l^2 e_l, \quad [h_j, c] = 0, \quad j, l = 1, ..., n$$

Problem 2.9. Show that $\langle H|M\rangle \geq \frac{1}{2}\hbar\omega$ for every $M \in \mathscr{S}$, where H is the Hamiltonian of the harmonic oscillator with one degree of freedom.

Problem 2.10. Let $q(t) = A\cos(\omega t + \alpha)$ be the classical trajectory of the harmonic oscillator with $m = 1$ and the energy $E = \frac{1}{2}\omega^2 A^2$, and let μ_α be the probability measure on $\mathbb{R}$ supported at the point $q(t)$. Show that the convex linear combination of the measures $\mu_\alpha, 0 \leq \alpha \leq 2\pi$, is the probability measure on $\mathbb{R}$ with the distribution function $\mu(q) = \frac{\theta\left(A^2 - q^2\right)}{\pi\sqrt{A^2 - q^2}}$, where $\theta(q)$ is the Heavyside step function.

Problem 2.11. Show that when $n \to \infty$ and $\hbar \to 0$ such that $\hbar\omega\left(n + \frac{1}{2}\right) = \frac{1}{2}\omega^2 A^2$ remains fixed, the envelope of the distribution function $|\psi_n(q)|^2$ on the interval $|q| \leq A$ coincides with the classical distribution function $\mu(q)$ from the previous problem. (Hint: Prove the integral representation

$$e^{-q^2} H_n(q) = \frac{2^{n+1}}{\sqrt{\pi}} \int_0^\infty e^{-y^2} y^n \cos\left(2qy - \frac{1}{2} n\pi\right) dy$$

and derive the asymptotic formula

$$\psi_n(q) = \sqrt{\frac{2}{\pi}} \frac{1}{\sqrt[4]{A^2 - q^2}} \cos\left\{\frac{\omega}{2\hbar}\left(A^2 \sin^{-1}\frac{q}{A} + q\sqrt{A^2 - q^2} - \frac{1}{2}A^2\pi\right) + O(1)\right\}$$

when $\hbar \to 0$ and $\hbar\left(n + \frac{1}{2}\right) = \frac{1}{2}\omega A^2, |q| < A$.)

Problem 2.12. Complete the proof of Theorem 2.1.

Problem 2.13 (The N-representation theorem). Let $\psi \in \mathscr{S}(\mathbb{R})$. Show that the L^2-convergent expansion $\psi = \sum_{n=0}^{\infty} c_n \psi_n$, where $c_n = (\psi, \psi_n)$, converges in $\mathscr{S}(\mathbb{R})$. (Hint: Use $N\psi_n = n\psi_n$.)

Problem 2.14. Show that the operators $E_{ij} = a_i^* a_j, i, j = 1, ..., n$, satisfy the commutation relations of the Lie algebra $\mathrm{sl}(n, \mathbb{C})$.

3.2.3 Quantization: Conceptual Questions

О случаях применения

(пока хз)

[023] Here, using the standard Euclidean metric on $\mathbb{R}^n$, we lowered the indices for Q^j.

Все-таки, почему скобка Пуассона должна переходить в коммутатор? В чем смысл этого? (!?!??!??!?)

(потом очень подробно отвечу, смысл этого пока так себе понимаю)

How to guess the way, how does canonical quantization work?

(great question, actually.... Maybe, answer is in Kiselev's style, that we have infinitesemal algebra, so we work on this level... I'll write later)

Why there are a lot of ways of quantization?

(??? I don't know??? a good question)

How does the method of canonical quantization (or other one) is related to the picture that we had some field (smooth distribution of matter) and now we have points (quantums)?

(??? I don't know??? a good question. so the problem is that this mathematics do not give us the intuitive picture (which one naively imagines))

3.2.4 Quantization: Advanced Features of Basic Methods

2.7. Holomorphic representation and Wick symbols.

Let

$$\ell^2 = \left\{ c = \{c_n\}_{n=0}^{\infty} : \|c\|^2 = \sum_{n=0}^{\infty} |c_n|^2 < \infty \right\}$$

be the Hilbert ℓ^2-space. The choice of an orthonormal basis $\{\psi_n\}_{n=0}^{\infty}$ for $L^2(\mathbb{R}, dq)$, given by the eigenfunctions (2.40) of the Schrodinger operator for the harmonic oscillator, establishes the Hilbert space isomorphism $L^2(\mathbb{R}, dq) \simeq \ell^2$,

$$L^2(\mathbb{R}, dq) \ni \psi = \sum_{n=0}^{\infty} c_n \psi_n \mapsto c = \{c_n\}_{n=0}^{\infty} \in \ell^2$$

where

$$c_n = (\psi, \psi_n) = \int_{-\infty}^{\infty} \psi(q)\psi_n(q)dq$$

since the functions ψ_n are real-valued. Using (2.39) we get

$$a^*\psi = \sum_{n=0}^{\infty} c_n a^*\psi_n = \sum_{n=0}^{\infty} \sqrt{n+1} c_n \psi_{n+1} = \sum_{n=1}^{\infty} \sqrt{n} c_{n-1}\psi_n, \quad \psi \in D(a^*)$$

and

$$a\psi = \sum_{n=0}^{\infty} c_n a\psi_n = \sum_{n=1}^{\infty} \sqrt{n} c_n \psi_{n-1} = \sum_{n=0}^{\infty} \sqrt{n+1} c_{n+1}\psi_n, \quad \psi \in D(a)$$

so that in ℓ^2 creation and annihilation operators a^* and a are represented by the following semi-infinite matrices:

$$a = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad a^* = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

As a result,

$$N = a^* a = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 2 & 0 & \cdots \\ 0 & 0 & 0 & 3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

so that the Hamiltonian of the harmonic oscillator is represented by a diagonal matrix,

$$H = \hbar\omega \left(N + \frac{1}{2} \right) = \operatorname{diag} \left\{ \frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \ldots \right\}$$

This representation of the Heisenberg commutation relations is called the representation by occupation numbers, and has the property that in this representation the Hamiltonian H of the harmonic operator is diagonal.

Another representation where H is diagonal is constructed as follows. Let $\mathscr{D}$ be the space of entire functions $f(z)$ with the inner product

$$(f, g) = \frac{1}{\pi} \int_{\mathbb{C}} f(z) \overline{g(z)} e^{-|z|^2} d^2 z \tag{2.44}$$

where $d^2 z = \frac{i}{2} dz \wedge d\bar{z}$ is the Lebesgue measure on $\mathbb{C} \simeq \mathbb{R}^2$. It is easy to check that $\mathscr{D}$ is a Hilbert space with the orthonormal basis

$$f_n(z) = \frac{z^n}{\sqrt{n!}}, \quad n = 0, 1, 2, \ldots$$

The correspondence

$$\ell^2 \ni c = \{c_n\}_{n=0}^{\infty} \mapsto f(z) = \sum_{n=0}^{\infty} c_n f_n(z) \in \mathscr{D}$$

establishes the Hilbert space isomorphism $\ell^2 \simeq \mathscr{D}$. The realization of a Hilbert space $\mathscr{H}$ as the Hilbert space $\mathscr{D}$ of entire functions is called a holomorphic representation. In the holomorphic representation,

$$a^* = z, \quad a = \frac{d}{dz}, \quad \text{and} \quad H = \hbar\omega \left(z \frac{d}{dz} + \frac{1}{2} \right)$$

and it is very easy to show that a^* is the adjoint operator to a. The mapping

$$\mathscr{H} \ni \psi = \sum_{n=0}^{\infty} c_n \psi_n \mapsto f(z) = \sum_{n=0}^{\infty} c_n f_n(z) \in \mathscr{D}$$

establishes the isomorphism between the coordinate and holomorphic representations. It follows from the formula for the generating function for Hermite-Tchebyscheff polynomials,

$$\sum_{n=0}^{\infty} H_n(q)\frac{z^n}{n!} = e^{2qz-z^2}$$

that the corresponding unitary operator $U : \mathscr{H} \to \mathscr{D}$ is an integral operator

$$U\psi(z) = \int_{-\infty}^{\infty} U(z,q)\psi(q)dq$$

with the kernel

$$U(z,q) = \sum_{n=0}^{\infty} \psi_n(q)f_n(z) = \sqrt[4]{\frac{m\omega}{\pi\hbar}} e^{\frac{m\omega}{2\hbar}q^2 - \left(\sqrt{\frac{m\omega}{\hbar}}q - \frac{1}{\sqrt{2}}z\right)^2} \tag{2.45}$$

Another useful realization is a representation in the Hilbert space $\overline{\mathscr{D}}$ of anti-holomorphic functions $f(\bar{z})$ on $\mathbb{C}$ with the inner product

$$(f,g) = \frac{1}{\pi}\int_{\mathbb{C}} f(\bar{z})\overline{g(\bar{z})}e^{-|z|^2}d^2z$$

given by

$$a^* = \bar{z}, \quad a = \frac{d}{d\bar{z}}.$$

Remark. Holomorphic and anti-holomorphic representations correspond to different choices of a complex polarization of the symplectic manifold $\mathbb{R}^2$. By definition, a complex polarization of a symplectic manifold $(\mathscr{M}, \omega)$ is an integrable distribution on $\mathscr{M}$ of complex Lagrangian subspaces of the complexified vector spaces $T_x\mathscr{M} \otimes_{\mathbb{R}} \mathbb{C}$. As the notion of real polarization, the notion of complex polarization plays a fundamental role in geometric quantization. In particular, holomorphic representation corresponds to the complex Lagrangian subspace in $T_x\mathbb{R}^2 \otimes_{\mathbb{R}} \mathbb{C} \simeq \mathbb{C}^2$ given by the equation $z = 0$, where z and $\bar{z}$ are complex coordinates on $\mathbb{C}^2$. (Note that here $\bar{z}$ is not a complex conjugate to z !) The equation $\bar{z} = 0$ defines a complex Lagrangian subspace which corresponds to the anti-holomorphic representation.

The anti-holomorphic representation is used to introduce the so-called Wick symbols of the operators. Namely, let A be an operator in $\overline{\mathscr{D}}$ which is a polynomial with constant coefficients in creation and annihilation operators a^* and a. Using the commutation relation (2.34), we can move all operators a^* to the left of the operators a, and represent A in the Wick normal form as follows:

$$A = \sum_{l,m} A_{lm}\,(a^*)^l\,a^m \tag{2.46}$$

By definition, the Wick symbol $A(\bar{z}, z)$ of the operator A is

$$A(\bar{z}, z) = \sum_{l,m} A_{lm}\bar{z}^l z^m \tag{2.47}$$

It is a restriction of a polynomial $A(v, z)$ in variables v and z to $v = \bar{z}$.
In order to define Wick symbols of bounded operators in $\overline{\mathscr{D}}$, we consider the family of coherent states (or Poisson vectors) $\Phi_v \in \overline{\mathscr{D}}, v \in \mathbb{C}$, defined by

$$\Phi_v(\bar{z}) = e^{v\bar{z}}, \quad z \in \mathbb{C}$$

They satisfy the properties

$$a\Phi_v = v\Phi_v \quad \text{and} \quad f(\bar{v}) = (f, \Phi_v), \quad f \in \overline{\mathscr{D}}, v \in \mathbb{C}. \tag{2.48}$$

Indeed, the first property is trivial, whereas the "reproducing property" immediately follows from the formula

$$\Phi_v(\bar{z}) = \sum_{n=0}^{\infty} f_n(v)\bar{f}_n(\bar{z}) \tag{2.49}$$

where $\bar{f}_n(\bar{z}) = \overline{f_n(z)}, n = 0, 1, 2, ...$, is the orthonormal basis for $\overline{\mathscr{D}}$.
We also have

$$(f, g) = \frac{1}{\pi}\int_{\mathbb{C}} (f, \Phi_v)\,\overline{(g, \Phi_v)}e^{-|v|^2}d^2v \tag{2.50}$$

Now for the operator A in the Wick normal form (2.46) we get, using the first property in (2.48),

$$\begin{aligned}(A\Phi_z, \Phi_{\bar{v}}) &= \sum_{l,m} A_{lm}\left((a^*)^l a^m\Phi_z, \Phi_{\bar{v}}\right) = \sum_{l,m} A_{lm}\left(a^m\Phi_z, a^l\Phi_{\bar{v}}\right)\\ &= A(v, z)\,(\Phi_z, \Phi_{\bar{v}})\,.\end{aligned}$$

Therefore,

$$A(v, z) = \frac{(A\Phi_z, \Phi_{\bar{v}})}{(\Phi_z, \Phi_{\bar{v}})} = e^{-vz}\,(A\Phi_z, \Phi_{\bar{v}})$$

since by the reproducing property, $(\Phi_z, \Phi_{\bar{v}}) = \Phi_z(v) = e^{vz}$.

Definition. The Wick symbol $A(\bar{z}, z)$ of a bounded operator A in the Hilbert space $\overline{\mathscr{D}}$ is a restriction to $v = \bar{z}$ of an entire function $A(v, z)$ in variables v and z, defined by

$$A(v, z) = e^{-vz}\,(A\Phi_z, \Phi_{\bar{v}})$$

In the next theorem, we summarize the properties of the Wick symbols.
Theorem 2.2. Wick symbols of the bounded operators on $\overline{\mathscr{D}}$ have the following properties.
(i) If $A(\bar{z}, z)$ is the Wick symbol of an operator A, then for the Wick symbol of the operator A^* we have $A^*(\bar{z}, z) = \overline{A(\bar{z}, z)}$ and

$$A^*(v, z) = \overline{A(\bar{z}, \bar{v})}$$

(ii) For $f \in \overline{\mathscr{D}}$,

$$(Af)(\bar{z}) = \frac{1}{\pi}\int_{\mathbb{C}} A(\bar{z}, v)f(\bar{v})e^{-v(\bar{v}-\bar{z})}d^2v$$

(iii) A real-analytic function $A(\bar{z}, z)$ is a Wick symbol of a bounded operator A in $\overline{\mathscr{D}}$ if and only if it is a restriction to $v = \bar{z}$ of an entire function $A(v, z)$ in variables v and z with the property that for every $f \in \overline{\mathscr{D}}$ the integral in part (ii) is absolutely convergent and defines a function in $\overline{\mathscr{D}}$.
(iv) If $A_1(\bar{z}, z)$ and $A_2(\bar{z}, z)$ are the Wick symbols of operators A_1 and A_2, then the Wick symbol of the operator $A = A_1A_2$ is given by

$$A(\bar{z}, z) = \frac{1}{\pi}\int_{\mathbb{C}} A_1(\bar{z}, v)A_2(\bar{v}, z)e^{-(v-z)(\bar{v}-\bar{z})}d^2v$$

Proof. We have

$$A^*(v,z) = e^{-vz}\,(A^*\Phi_z, \Phi_{\bar v}) = e^{-vz}\,(\Phi_z, A\Phi_{\bar v}) = e^{-vz}\overline{(A\Phi_{\bar v}, \Phi_z)} = \overline{A(\bar z, \bar v)},$$

which proves (i). To prove (ii), we use the reproducing property to get

$$(Af)(\bar z) = (Af, \Phi_z) = (f, A^*\Phi_z) = \frac{1}{\pi}\int_{\mathbb{C}} f(\bar v)\overline{(A^*\Phi_z)\,(\bar v)}e^{-|v|^2}d^2v$$

Using the reproducing property once again we have

$$(A^*\Phi_z)\,(\bar v) = (A^*\Phi_z, \Phi_v) = A^*(\bar v, z)\,(\Phi_z, \Phi_v) = \overline{e^{v\bar z}A(\bar z, v)},$$

which proves (ii). Property (iii) follows from the definition and the uniform boundness principle, which is needed to show that the operator A on $\overline{\mathscr{D}}$,
defined by the integral in (ii), is bounded. We leave the standard details to the reader. To prove (iv), by using (2.50) and (i) we get

$$\begin{aligned} A(\bar z, z) &= e^{-|z|^2}\,(A_1A_2\Phi_z, \Phi_z) = e^{-|z|^2}\,(A_2\Phi_z, A_1^*\Phi_z) \\ &= \frac{1}{\pi}\int_{\mathbb{C}} (A_2\Phi_z, \Phi_v)\,\overline{(A_1^*\Phi_z, \Phi_v)}e^{-\left(|v|^2+|z|^2\right)}d^2v \\ &= \frac{1}{\pi}\int_{\mathbb{C}} A_1(\bar z, v)A_2(\bar v, z)e^{-(v-z)(\bar v-\bar z)}d^2v \end{aligned}$$

Remark. Properties (i) and (iv) remain valid for the polynomials in a^* and a - operators of the form (2.46).

A matrix symbol $\tilde A(\bar z, z)$ of a bounded operator A in the Hilbert space $\overline{\mathscr{D}}$ is a restriction to $v = \bar z$ of an entire function $\tilde A(v, z)$ in variables v and z, defined by the following absolutely convergent series:

$$\tilde A(v,z) = \sum_{m,n=0}^{\infty} \left(A\bar f_m, \bar f_n\right) f_n(v)f_m(z) \tag{2.51}$$

The matrix and Wick symbols are related as follows.
Lemma 2.4. For a bounded operator A in the Hilbert space $\overline{\mathscr{D}}$,

$$\tilde A(v,z) = e^{vz}A(v,z)$$

Proof. Using (2.49) we get

$$\begin{aligned} \tilde A(v,z) &= \frac{1}{\pi}\sum_{m,n=0}^{\infty} f_n(v)f_m(z)\int_{\mathbb{C}} \left(A\bar f_m\right)(\bar u)f_n(u)e^{-|u|^2}d^2u \\ &= \frac{1}{\pi}\int_{\mathbb{C}} (A\Phi_z)\,(\bar u)\overline{\Phi_{\bar v}(\bar u)}e^{-|u|^2}d^2u = (A\Phi_z, \Phi_{\bar v}) = e^{vz}A(v,z) \end{aligned}$$

Changing the order of summation and integration is justified by the absolute convergence.
Corollary 2.3. If $\tilde A_1(\bar z, z)$ and $\tilde A_2(\bar z, z)$ are matrix symbols of operators A_1 and A_2, then the matrix symbol of the operator $A = A_1A_2$ is given by

$$\tilde A(\bar z, z) = \frac{1}{\pi}\int_{\mathbb{C}} \tilde A_1(\bar z, v)\tilde A_2(\bar v, z)e^{-|v|^2}d^2v$$

Proof. The proof immediately follows from part (iv) of Theorem 2.2 and Lemma 2.4.

It is straightforward to generalize these constructions to n degrees of freedom. The Hilbert space $\mathscr{D}_n$ defining the holomorphic representation is
the space of entire functions $f(\boldsymbol{z})$ of n complex variables $\boldsymbol{z} = (z_1, ..., z_n)$ with the inner product

$$(f, g) = \frac{1}{\pi^n} \int_{\mathbb{C}^n} f(\boldsymbol{z}) \overline{g(\boldsymbol{z})} e^{-|\boldsymbol{z}|^2} d^{2n}\boldsymbol{z} < \infty$$

where $|\boldsymbol{z}|^2 = z_1^2 + \cdots + z_n^2$ and $d^{2n}\boldsymbol{z} = d^2 z_1 \cdots d^2 z_n$ is the Lebesgue measure on $\mathbb{C}^n \simeq \mathbb{R}^{2n}$. The functions

$$f_m(\boldsymbol{z}) = \frac{z_1^{m_1} ... z_n^{m_n}}{\sqrt{m_1! ... m_n!}}, \quad m_1, ..., m_n = 0, 1, 2, ...$$

where $\boldsymbol{m} = (m_1, ..., m_n)$ is a multi-index, form an orthonormal basis for $\mathscr{D}_n$. Corresponding creation and annihilation operators are given by

$$a_j^* = z_j, \quad a_j = \frac{\partial}{\partial z_j}, \quad j = 1, ..., n$$

The Hilbert space $\overline{\mathscr{D}}_n$ of anti-holomorphic functions $f(\overline{\boldsymbol{z}})$ on $\mathbb{C}^n$ is defined by the inner product

$$(f, g) = \frac{1}{\pi^n} \int_{\mathbb{C}^n} f(\overline{\boldsymbol{z}}) \overline{g(\overline{\boldsymbol{z}})} e^{-|\boldsymbol{z}|^2} d^{2n}\boldsymbol{z} < \infty, \tag{2.52}$$

and the creation and annihilation operators are given by

$$a_j^* = \bar{z}_j, \quad a_j = \frac{\partial}{\partial \bar{z}_j}, \quad j = 1, ..., n.$$

The coherent states are $\Phi_{\boldsymbol{v}}(\overline{\boldsymbol{z}}) = e^{\boldsymbol{v}\overline{\boldsymbol{z}}}$, where $\boldsymbol{v}\overline{\boldsymbol{z}} = v_1\bar{z}_1 + \cdots + v_n z_n$, and satisfy the reproducing property

$$f(\overline{\boldsymbol{v}}) = (f, \Phi_{\boldsymbol{v}}), \quad f \in \overline{\mathscr{T}}_n, \quad \boldsymbol{v} \in \mathbb{C}^n$$

The Wick symbol $A(\overline{\boldsymbol{z}}, \boldsymbol{z})$ of a bounded operator A on $\overline{\mathscr{D}}_n$ is defined as a restriction to $\boldsymbol{v} = \overline{\boldsymbol{z}}$ of an entire function $A(\boldsymbol{v}, \boldsymbol{z})$ of $2n$ variables $\boldsymbol{v} = (v_1, ..., v_n)$ and $\boldsymbol{z} = (z_1, ..., z_n)$, given by

$$A(\boldsymbol{v}, \boldsymbol{z}) = e^{-\boldsymbol{v}\boldsymbol{z}} (A\Phi_{\boldsymbol{z}}, \Phi_{\overline{\boldsymbol{v}}}).$$

We have

$$(Af)(\overline{\boldsymbol{z}}) = \frac{1}{\pi^n} \int_{\mathbb{C}^n} A(\overline{\boldsymbol{z}}, \boldsymbol{v}) f(\overline{\boldsymbol{v}}) e^{-\boldsymbol{v}(\overline{\boldsymbol{v}} - \overline{\boldsymbol{z}})} d^{2n}\boldsymbol{v}, \quad f \in \overline{\mathscr{D}}_n$$

and the Wick symbol $A(\bar{z}, z)$ of the operator $A = A_1 A_2$ is given by

$$A(\bar{z}, \boldsymbol{z}) = \frac{1}{\pi^n} \int_{\mathbb{C}^n} A_1(\overline{\boldsymbol{z}}, \boldsymbol{v}) A_2(\overline{\boldsymbol{v}}, \boldsymbol{z}) e^{-(\boldsymbol{v} - \boldsymbol{z})(\overline{\boldsymbol{v}} - \overline{\boldsymbol{z}})} d^{2n}\boldsymbol{v}$$

where $A_1(\overline{\boldsymbol{z}}, \boldsymbol{z})$ and $A_2(\overline{\boldsymbol{z}}, \boldsymbol{z})$ are the Wick symbols of the operators A_1 and A_2.

The matrix symbol $\tilde{A}(\overline{\boldsymbol{z}}, \boldsymbol{z})$ of a bounded operator A on $\overline{\mathscr{D}}_n$ is defined as a restriction to $\boldsymbol{v} = \overline{\boldsymbol{z}}$ of an entire function $\tilde{A}(\boldsymbol{v}, \boldsymbol{z})$ of $2n$ variables $\boldsymbol{v} = (v_1, ..., v_n)$ and $\boldsymbol{z} = (z_1, ..., z_n)$, given by the absolutely convergent series

$$\tilde{A}(\boldsymbol{v}, \boldsymbol{z}) = \sum_{\boldsymbol{k}, \boldsymbol{m} = 0}^{\infty} \left(A\bar{f}_{\boldsymbol{k}}, \bar{f}_{\boldsymbol{m}}\right) f_{\boldsymbol{m}}(\boldsymbol{v}) f_{\boldsymbol{k}}(\boldsymbol{z})$$

where $\boldsymbol{k} = (k_1, ..., k_n), \boldsymbol{m} = (m_1, ..., m_n)$ are multi-indices, and $\bar{f}_{\boldsymbol{m}}(\overline{\boldsymbol{z}}) = \overline{f_m(\boldsymbol{z})}$. The matrix and Wick symbols of a bounded operator A are related by

$$\tilde{A}(\boldsymbol{v}, \boldsymbol{z}) = e^{\boldsymbol{v}\boldsymbol{z}} A(\boldsymbol{v}, \boldsymbol{z})$$

Remark. The anti-holomorphic representation is very useful in quantum mechanics and especially in quantum field theory, where it is called holomorphic representation (with respect to the variables $\overline{\boldsymbol{z}}$). Slightly abusing terminology, in Part 2 we will also call it holomorphic representation.

Problem 2.15. Find an explicit formula for the unitary operator establishing the Hilbert space isomorphism $\overline{\mathscr{D}}_n \simeq L^2(\mathbb{R}^n, d^n\boldsymbol{q})$.

Problem 2.16. Prove that for the bounded operator A the functions $A(\boldsymbol{v}, \boldsymbol{z})$ and $\tilde{A}(\boldsymbol{v}, \boldsymbol{z})$ are entire functions of $2n$ variables.

Problem 2.17. Let A be a trace class operator on $\overline{\mathscr{D}}_n$ with the Wick symbol $A(\bar{z}, \boldsymbol{z})$. Prove that

$$\operatorname{Tr} A = \frac{1}{\pi^n} \int_{\mathbb{C}^n} A(\bar{z}, \boldsymbol{z}) e^{-|\boldsymbol{z}|^2} d^{2n}\boldsymbol{z}$$

Problem 2.18. Show that the Wick symbol $A(\bar{z}, z)$ of the product $A = A_l ... A_1$ is given by

$$A(\bar{z}, z) = \frac{1}{\pi^l} \int_{\mathbb{C}^l} A_l(\bar{z}, z_{l-1}) ... A_1(\bar{z}_1, z) \exp\left\{ \sum_{k=1}^{l} \bar{z}_k (z_{k-1} - z_k) \right\} d^2 z_1 ... d^2 z_{l-1}$$

where $z_0 = z_l = z, \bar{z}_l = \bar{z}$, and $A_k(\bar{z}, z)$ are the Wick symbols of the operators A_k.

3.2.5 Quantization by the Bohr–Sommerfeld Rule (?)

(this also works as quantization, but currently I have no idea how this fits into the modern physic world, so it is a conceptual question, what is it?)

3.3 Second Quantization

Second quantization is conceptually important topic, thus I have a subsection about it, not subsubsection. Basically, it answers question "okay, we have Schrodinger equation, but what it there are a lot of electrons and they interact one with another with some law"? Understanding exactly of this method will allow one to use QM for something really meaningful, and not for some one-particle conceptually simple model.

3.3.1 Basics of Second Quantization

Обсудим подробно вторичное квантование

Origin of creation and annihilation operators

(we have Schrodinger equation. okay. why we are introducing operators????? answer this question!)

Second quantization as a magic teleportation of a state from one to another

(two particle just stop to exist, then new two particles appear. discuss this)

Coulomb interaction

(discuss how exchange of virtual photon looks like. this is also in the note on QFT)

вкратце теория

(левитов шитов начало)

Рассмотрим вначале систему бозе-частиц, каждая из которых может находиться в одном из состояний $\psi_i(x), i = 1, 2, ...$ Многочастичная волновая функция задается в представлении чисел заполнения, указывающем сколько частиц занимают каждое из состояний $\psi_i(x)$.

В обозначениях Дирака такие состояния могут быть записаны как $|..., N_{i-1}, N_i, N_{i+1}, ...\rangle$, где числа заполнения N_i принимают произвольные целые неотрицательные значения, $N_i = 0, 1, ...$ Канонические операторы рождения и уничтожения a_i^+ и a_i вводятся следующим образом:

$$a_i |..., N_i, N_{i+1}, ...\rangle = \sqrt{N_i} |..., N_i - 1, N_{i+1}, ...\rangle$$
$$a_i^+ |..., N_i, N_{i+1}, ...\rangle = \sqrt{N_i + 1} |..., N_i + 1, N_{i+1}, ...\rangle$$

Нетрудно проверить, что выполняются коммутационные соотношения:

$$\left[a_i, a_j^+\right] = a_i a_j^+ - a_j^+ a_i = \delta_{ij}; \quad [a_i, a_j] = \left[a_i^+, a_j^+\right] = 0$$

Далее, вводятся ψ -операторы:

$$\widehat{\psi}(x) = \sum_i \widehat{a}_i \psi_i(x); \quad \widehat{\psi}^+(x) = \sum_i \widehat{a}_i^+ \psi_i^*(x)$$

Функции $\psi_i(x)$ выбирают таким образом, чтобы они образовывали полную ортонормированную систему.

При этом коммутационные соотношения ψ -операторов оказываются следующими:

$$\left[\widehat{\psi}(x), \widehat{\psi}^+(x')\right] = \delta(x - x'), \quad \left[\widehat{\psi}(x), \widehat{\psi}(x')\right] = \left[\widehat{\psi}^+(x), \widehat{\psi}^+(x')\right] = 0$$

В случае ферми-статистики представление чисел заполнения, а также операторы рождения и уничтожения, их коммутационные соотношения и ψ -операторы вводятся сходным образом.

Остановимся на отличиях бозевского и фермиевского вторичного квантования.

Во-первых, в силу принципа Паули, числа заполнения N_i принимают всего два значения: $N_i = 0, 1$.

Поэтому канонические операторы a_i и a_i^+ действуют так:

$$a_i |..., N_i, N_{i+1}, ...\rangle = \begin{cases} |..., 0, N_{i+1}, ...\rangle & \text{при } N_i = 1 \\ 0 & \text{при } N_i = 0 \end{cases}$$
$$a_i^+ |..., N_i, N_{i+1}, ...\rangle = \begin{cases} 0 & \text{при } N_i = 1 \\ |..., 1, N_{i+1}, ...\rangle & \text{при } N_i = 0 \end{cases}$$

Во-вторых, антисимметрия многочастичного состояния по отношению к перестановке частиц приводит к антикоммутативности a_i и a_j^+ :

$$\left[a_i^+, a_j\right]_+ = a_i^+ a_j + a_j a_i^+ = \delta_{ij}, \quad [a_i, a_j]_+ = \left[a_i^+, a_j^+\right]_+ = 0$$

Для ψ -операторов (1.3) соотношения антикоммутативности выглядят так:

$$\left[\widehat{\psi}(x), \widehat{\psi}^+(x')\right]_+ = \delta(x - x'), \quad \left[\widehat{\psi}(x), \widehat{\psi}(x')\right]_+ = \left[\widehat{\psi}^+(x), \widehat{\psi}^+(x')\right]_+ = 0$$

Удобство представления вторичного квантования заключается в том, связь между одно- и многочастичной задачами на языке ψ -операторов оказывается весьма простой.

Например, нетрудно проверить, что гамильтониан системы невзаимодействующих бозе- или ферми-частиц, имеющих массу m и движущихся в потенциале $U(\mathbf{r})$, записывается так:

$$\widehat{\mathcal{H}} = \int \left(-\frac{\hbar^2}{2m} \widehat{\psi}^{+}(\mathbf{r}) \nabla^2 \hat{\psi}(\mathbf{r}) + \widehat{\psi}^{+}(\mathbf{r}) \hat{\psi}(\mathbf{r}) U(\mathbf{r}) \right) d^3 r$$

А если частицы взаимодействуют по закону $V(\mathbf{r}_1 - \mathbf{r}_2)$, то гамильтониан нужно просто дополнить членом

$$\widehat{\mathcal{H}}_{\text{int}} = \frac{1}{2} \iint \widehat{\psi}^{+}(\mathbf{r}_1) \widehat{\psi}^{+}(\mathbf{r}_2) V(\mathbf{r}_1 - \mathbf{r}_2) \widehat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) d^3 r_1 d^3 r_2$$

Вторично квантованный оператор плотности частиц $\hat{\rho}(\mathbf{r}) = \widehat{\psi}^{+}(\mathbf{r}) \widehat{\psi}(\mathbf{r})$ является многочастичным эквивалентом одночастичного выражения $|\psi(\mathbf{r})|^2$ для плотности вероятности.

Интеграл от $\hat{\rho}(\mathbf{r})$, взятый по всему пространству, есть оператор полного числа частиц в системе

$$\widehat{N} = \int \widehat{\psi}^{+}(\mathbf{r}) \hat{\psi}(\mathbf{r}) d^3 r$$

Подчеркнем, что все операторы (1.8) – (1.10) в представлении вторичного квантования имеют один и тот же вид и для фермионов, и для бозонов.

Examples of second quantization

Second quantization of particle operator

Your particle density operator $n(\mathbf{x}) = \sum_\alpha \delta(\mathbf{x} - \mathbf{x}_\alpha)$ is in first-quantized form and $\hat{n}(\mathbf{x}) = \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x})$ is second-quantized.

When a general one-body operator is written in first-quantized form $J = \sum_\alpha J(\mathbf{x}_\alpha)$, the secondquantized form is:

$$\begin{aligned} \hat{J} &\equiv \sum_{rs} \langle r|J|s\rangle \hat{c}_r^\dagger \hat{c}_s \\ &= \sum_{rs} \int d\mathbf{x}' \psi_r^*(\mathbf{x}') J(\mathbf{x}') \psi_s(\mathbf{x}') \hat{c}_r^\dagger \hat{c}_s \\ &= \int d\mathbf{x}' \hat{\psi}^\dagger(\mathbf{x}') J(\mathbf{x}') \hat{\psi}(\mathbf{x}') \end{aligned}$$

The last equality follows from $\hat{\psi}(\mathbf{x}) \equiv \sum_s \psi_s(\mathbf{x}) \hat{c}_s$. In the case of the particle density operator:

$$\begin{aligned} \hat{n}(\mathbf{x}) &= \int d\mathbf{x}' \hat{\psi}^\dagger(\mathbf{x}') \delta(\mathbf{x} - \mathbf{x}') \hat{\psi}(\mathbf{x}') \\ &= \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}) \end{aligned}$$

Please let me know if you'd like more detail on any of these steps. For somewhat relevant discussion on the relation between first and second-quantized operators, see my answer here: Second quantization. In that answer I only considered the two body interaction operator in detail. I could do the same for (simpler) one body operators if it'd be of help.

Мы понимаем, что в классической механике у нас точка, а в квантовой - волновая функция, то есть координата не определена. Как это следует из определения квантования операторов? (!??!?!?)

(додумаю, интересный и концептуально важный вопрос, но для задач это не нужно знать.)

3.3.2 Second Quantization: Advanced Properties, Other Questions

Concept of canonical transformations for second-quantized operators

Остановимся теперь на важном понятии канонического преобразования и на том, как эти преобразования выглядят в представлении вторичного квантования.

Напомним, что в классической механике канонические преобразования фазового пространства $(p, q) \to (p', q')$ вводятся с помощью скобок Пуассона $\{\ldots\}$, причем роль

этих преобразований заключается в том, что они сохраняют гамильтонову форму уравнений движения: $\dot{p} = \{p, H\}, \dot{q} = \{q, H\}$.

В квантовой механике роль скобок Пуассона переходит к коммутаторам.

(Например, в представлении Гейзенберга уравнения движения имеют вид $i\hbar\partial_t \widehat{A} = [\widehat{A}, \widehat{\mathcal{H}}].$) Поэтому каноническими называют преобразования физических величин, сохраняющие коммутационные соотношения операторов.

Как и в классической механике, канонические преобразования важны, поскольку они сохраняют форму уравнений движения.

Подобрав каноническое преобразование, часто возможно перейти от взаимодействующих частиц к невзаимодействующим квазичастицам.

Наиболее часто рассматривают линейные преобразования канонических операторов (бозонов или фермионов)

$$\tilde{a}_i = \sum_j \left(U_{ij} a_j + V_{ij} a_j^+\right), \quad \tilde{a}_i^+ = \sum_j \left(V_{ij}^* a_j + U_{ij}^* a_j^+\right)$$

называемые преобразованиями Боголюбова.

Одной из часто встречающихся задач является отыскание спектра и собственных состояний гамильтониана, квадратичного по операторам рождения и уничтожения.

Нетрудно проверить, что произвольный гамильтониан такого вида может быть приведен к диагональной форме с помощью соответствующим образом подобранного преобразования (1.11):

$$\widehat{\mathcal{H}} = \sum_{ij} h_{ij}^{(1)} a_i^+ a_j + h_{ij}^{(2)} a_i a_j + \text{h.c.} = \sum_i \varepsilon_i \tilde{a}_i^+ \tilde{a}_i + \langle 0|\widehat{\mathcal{H}}|0\rangle$$

Энергии ε_i дают спектр квазичастиц, а константа $\langle 0|\widehat{\mathcal{H}}|0\rangle$ в правой части представляет собой так называемую энергию нулевых колебаний.

Преобразования (1.11) являются каноническими, если они сохраняют коммутационные соотношения

$$[a_i, a_j]_\pm = 0, \quad \left[a_i, a_j^+\right]_\pm = \delta_{ij}$$

Соответствующие условия на матрицы U и V в (1.11) в общем случае выглядят так:

$$U_{ki} V_{kj} \pm V_{ki} U_{kj} = 0, \quad U_{ki}^* U_{kj} \pm V_{ki}^* V_{kj} = \delta_{ij}$$

где знак «+» соответствует случаю ферми-статистики, а знак -» - случаю бозестатистики.

Структура преобразований (1.11) для бозе-операторов видна уже в простейшем случае одной бозонной степени свободы (примером является квантово-механический осциллятор).

При этом U и V -не матрицы, а числа, и имеется всего два простейших однородных канонических преобразования:

$$\begin{array}{ll} \tilde{a} = \operatorname{ch}\lambda a + \operatorname{sh}\lambda a^+ & \tilde{a} = e^{i\varphi}\tilde{a} \\ \widetilde{a}^+ = \operatorname{sh}\lambda a + \operatorname{ch}\lambda a^+ & \widetilde{a}^+ = e^{-i\varphi}\widetilde{a}^+ \end{array}$$

где λ и φ -вещественные параметры.

Более обшие преобразования представляют собой произведение (композищию) преобразований (1.15).

В случае же ферми-статистики линейные канонические преобразования задаются сходным образом.

Для одной фермионной степени свободы все линейные канонические преобразования исчерпываются сопряжением, $\tilde{a} = a^+, \tilde{a}^+ = a$, и умножением на фазовый множитель, $\tilde{a} = e^{i\varphi}a^+, \tilde{a}^+ = e^{-i\varphi}a$, а преобразования более общего вида в этом случае оказываются нелинейными - см. задачу 3.

Более общие линейные преобразования возникают в системе из двух фермионов, например,

$$\begin{array}{ll} \tilde{a} = \cos\theta a - \sin\theta b^+ & \tilde{a}^+ = \cos\theta a^+ - \sin\theta b \\ \widetilde{b}^+ = \sin\theta a + \cos\theta b^+ & \tilde{b} = \sin\theta a^+ + \cos\theta b \end{array}$$

где θ -параметр.

Интересно, что первое из бозонных преобразований (1.15) есть псевдоевклидово вращение, то есть не что иное, как преобразование Лоренца с быстротой λ в двумерном пространстве -времени, в то время как для фермионов возникают преобразования вида (1.16), соответствующие вращению евклидова пространства.

Возможные канонические преобразования не исчерпываются однородными линейными преобразованиями.

Иногда бывают полезны неоднородные линейные преобразования (как в задаче 6) или даже нелинейные преобразования (см. задачу 3, а также раздел 1.4).

Часто встречаюшаяся разновидность линейных канонических преобразований фурье-преобразование ψ -операторов:

$$\widehat{\psi}(\mathbf{r}) = \int e^{i\mathbf{pr}}\widehat{a}_{\mathbf{p}}\frac{d^3p}{(2\pi)^3}, \quad \widehat{\psi}^+(\mathbf{r}) = \int e^{-i\mathbf{pr}}\widehat{a}^+_{\mathbf{p}}\frac{d^3p}{(2\pi)^3}$$

Принято выбирать нормировку операторов $\widehat{a}_{\mathbf{p}}$ и $\widehat{a}^+_{\mathbf{p}}$ так, чтобы

$$\left[\hat{a}_{\mathbf{p}_1}, \widehat{a}^+_{\mathbf{p}_2}\right]_{\pm} = (2\pi)^3\delta^{(3)}\left(\mathbf{p}_1 - \mathbf{p}_2\right)$$

Такой выбор согласуется с определениями (1.4) и (1.7).

Имеется важный для теории твердого тела круг задач, когда ψ -операторы или другие величины заданы на решетке. Фурье-преобразование (1.17) нетрудно распространить на этот случай, заметив, что если r пробегает узлы некоторой решетки, то $\mathbf{p}$ изменяется внутри периода обратной решетки (или, иначе говоря, внутри зоны Бриллюэна). Скажем, в одном измерении решетка есть $r_n = an$, а зона Бриллюэна это отрезок $-\pi/a < p < \pi/a$.

Other, conceptual questions about second quantization

О названии вторичного квантования

(почему это может быть похоже на то, что квантуем дважды???? пока не так понимаю)

О случаях применения вторичного квантования

(write that in QFT, in cond matter there are a lot of them! it is very used.)

Second quantization in density matrix formalism

(before I wrote only about the wave function, now, how to do the same if I describe the system by the density matrix? I don't know)

Is it possible to work with wave function for the models that are usually described in second quantized form?

(??? currently, I have no idea how to do it. maybe there is absolutely no sense in doing it, but even in terms of formalism, I am not sure at all, how to get back to WF formalism. I'll write it here)

How to deduce second quantization if it wasn't discovered?

(????? a very good question!!!)

How conceptually fermionic operators can appear from bosonic ones?

(??? also, it should be explained!!!)

3.4 Quantization: Special Methods

3.4.1 Quantization of Constrained Systems

(по идее просто лекции Дирака почитаю внимательно, там по идее теория, которая тут в страниц 40 должна уложиться.)

3.4.2 Quantization on Manifolds and in Other Coordinates (?)

(не знаю, есть магистерская работа про это, мб пойму когда-то)

3.4.3 Quantization of Fields and Space: Introduction

(про поля - отслыка в КТП, важное понимание для него. про пространство - отсылка в кв космологию, тоже по идее многое про это написано.)

О квантовании дираковского поля

О квантовании векторного поля

О квантовании плоского пространства (????)

О квантовании гравитации

(отдельные книги про это, так что просто коротко укажу. Скорее всего после записи отдельного это в отдельной записи.)

3.5 Density Matrix Formalism of QM

(!!! I'll write soon, since it is a very important basic concept)

3.5.1 Evolution of a Density Matrix

Evolution of a Density Matrix by Tokmakoff

The equation of motion for the density matrix follows naturally from the definition of ρ and the time-dependent Schrödinger equation.

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= \frac{\partial}{\partial t}[|\psi\rangle\langle\psi|] \\ &= \left[\frac{\partial}{\partial t}|\psi\rangle\right]\langle\psi| + |\psi\rangle\frac{\partial}{\partial t}\langle\psi| \\ &= \frac{-i}{\hbar}H|\psi\rangle\langle\psi| + \frac{i}{\hbar}|\psi\rangle\langle\psi|H \\ &= \frac{-i}{\hbar}[H,\rho]\end{aligned}$$

Equation 5.2.4 is the Liouville-Von Neumann equation. It is isomorphic to the Heisenberg equation of motion, since ρ is also an operator. The solution to Equation 5.2.4 is

$$\rho(t) = U\rho(0)U^\dagger$$

This can be demonstrated by first integrating Equation 5.2.4 to obtain

$$\rho(t) = \rho(0) - \frac{i}{\hbar}\int_0^t d\tau[H(\tau),\rho(\tau)]$$

If we expand Equation 5.2.6 by iteratively substituting into itself, the expression is the same as when we substitute

$$U = \exp_+\left[-\frac{i}{\hbar}\int_0^t d\tau H(\tau)\right]$$

into Equation 5.2.5 and collect terms by orders of $H(\tau)$.

Note that Equation 5.2.5 and the cyclic invariance of the trace imply that the time-dependent expectation value of an operator can be calculated either by propagating the operator (Heisenberg) or the density matrix (Schrödinger or interaction picture):

$$\begin{aligned}\langle\hat{A}(t)\rangle &= \mathrm{Tr}[\hat{A}\rho(t)] \\ &= \mathrm{Tr}\left[\hat{A}U\rho_0U^\dagger\right] \\ &= \mathrm{Tr}\left[\hat{A}(t)\rho_0\right]\end{aligned}$$

For a time-independent Hamiltonian it is straightforward to show that the density matrix elements evolve as

$$\begin{aligned}\rho_{nm}(t) &= \langle n|\rho(t)|m\rangle \\ &= \langle n|U\,|\psi_0\rangle\,\langle\psi_0|\,U^\dagger|m\rangle \\ &= e^{-i\omega_{nm}(t-t_0)}\rho_{nm}\,(t_0)\end{aligned}$$

From this we see that populations, $\rho_{mn}(t) = \rho_{nm}\,(t_0)$, are time-invariant, and coherences oscillate at the energy splitting ω_{nm}

3.5.2 Density Matrix Formalism: Examples of Applications

(see articles about it)

3.6 Schrodinger Equation

Here, we will discuss Schrodinger equation in detail.

One can ask, why such fundamental equation is after so many theory? This is because this part focuses on fundamental quantum mechanics, and Schrodinger equation is not the only one topic from fundamental point of view. From the point of view of solving some ideologically trivial, but mathematically not so obvious problems, it is indeed the central part. This is why it is first one in the first part of this nore/

3.6.1 Schrodinger Equation: Essential Properties for Everyone

(of course, this should be rewritten. I'll do it with some little practice)

Typical method of dealing with 1D Schrodinger equation

(this is the long and extended version of what is written in the first part)
(write that we join the derivative)

Уравнение Шредингера в импульсном представлении

Чтобы записать уравнение Шрёдингера в импульсном представлении, необходимо его спроектировать на бра-вектор $\langle \boldsymbol{p}|$, то есть рассмотреть $\langle \boldsymbol{p}|\hat{H}|\psi\rangle = E\langle \boldsymbol{p}|\psi\rangle$. Кинетическая энергия в таком случае запишется тривиально -этот оператор в импульсном представлении:

$$\left\langle \boldsymbol{p} \left| \frac{\hat{p}^2}{2m} \right| \psi \right\rangle = \frac{\boldsymbol{p}^2}{2m}\psi(\boldsymbol{p})$$

Потенциальная энергия не является диагональным оператором; поэтому нам пригодятся её матричные элементы в этом базисе.

Стандартный способ перехода между представлениями - вставление "разложения единиц" по базису, в котором мы знаем как действует оператор, в данном случае - в координатном базисе:

$$\langle \boldsymbol{p}|U(\hat{x})|\boldsymbol{p}'\rangle = \langle \boldsymbol{p}|U(\hat{\boldsymbol{x}}) \underbrace{\int d\boldsymbol{x}|\boldsymbol{x}\rangle\langle \boldsymbol{x}|}_{\mathbb{1}} |\boldsymbol{p}'\rangle = \int d\boldsymbol{x}U(\boldsymbol{x})\langle \boldsymbol{p}|\boldsymbol{x}\rangle \langle \boldsymbol{x}|\boldsymbol{p}'\rangle = \int d\boldsymbol{x}U(\boldsymbol{x})e^{-i(p-p')x} = U_{\boldsymbol{p}-\boldsymbol{p}'}$$

из чего мы заключаем, что эти матричные элементы тождественно совпадают с преобразованием Фурье от потенциала.

В таком случае, потенциальная энергия записывается в импульсном представлении в следующем виде:

$$\langle \boldsymbol{p}|U(\hat{\boldsymbol{x}})|\psi\rangle = \langle \boldsymbol{p}|U(\hat{\boldsymbol{x}}) \underbrace{\int (d\boldsymbol{p}') |\boldsymbol{p}'\rangle \langle \boldsymbol{p}'|}_{\hat{\mathbb{1}}} |\psi\rangle = \int (d\boldsymbol{p}')\, U_{\boldsymbol{p}-\boldsymbol{p}'}\psi(\boldsymbol{p}'),$$

где введено удобное обозначение $(d\boldsymbol{p}) \equiv d^d\boldsymbol{p}/(2\pi)^d$. Полученный объект называется свёрткой двух функций.

(?? это та самая свертка??)

Таким образом, уравнение Шрёдингера в импульсном представлении записывается в следующем виде:

$$\frac{p^2}{2m}\psi(\boldsymbol{p}) + \int (d\boldsymbol{p}')\,\psi(\boldsymbol{p}')\,U_{p-p'} = E\psi(\boldsymbol{p})$$

Таким образом, в импульсном представлении уравнение Шрёдингера уже интегральное, и иногда его оказывается решать проще.

(?? когда??)

Обсудим методы решения его, а также пример с мелкой ямой - одним из ключевых тому примеров.

Из общих рассуждений мы понимаем, что масштаб волновой функции в координатном представлении - большой масштаб $\kappa^{-1} \gg a$ -что из соотношения неопределённостей означает, что в импульсном представлении, напротив, волновая функция $\psi(p)$ является локализованной вблизи нуля на малом масштабе $\sim \kappa$. С другой стороны, масштаб $U(\boldsymbol{x})$ -это $a \ll \kappa^{-1}$; в свою очередь, масштаб $U_{p-p'}$ -это большой масштаб a^{-1}. Благодаря большой разнице в масштабах, в свёртке $\int (d\boldsymbol{p}')\,\psi(\boldsymbol{p}')\,U_{\boldsymbol{p}-\boldsymbol{p}'}$ основной вклад в интеграл приходит с $|\boldsymbol{p}'| \lesssim \kappa$, на котором функция $U_{\boldsymbol{p}-\boldsymbol{p}'}$ меняется слабо - поэтому

приближённому уравнению:

$$\frac{p^2}{2m}\psi(\boldsymbol{p}) + U_p \int (d\boldsymbol{p}')\,\psi(\boldsymbol{p}') = E\psi(\boldsymbol{p}) \to \psi(\boldsymbol{p}) = -\frac{U_{\boldsymbol{p}}}{-E + \frac{p^2}{2m}} \int (d\boldsymbol{p}')\,\psi(\boldsymbol{p}')$$

(отметим, что поскольку мы имеем дело с ямой, то потенциал $U(x) < 0$; и поскольку мы имеем дело со связанным состоянием, то $E = -|E| < 0$).

Данное уравнение - алгебраическое, ведь в правой части стоит интеграл от волновой функции, который является константой.

Последнее упрошение можно сделать, заметив, что в произведении перед интегралом, Опять-таки, $U_{\boldsymbol{p}}$ является медленной огибающей, а $(|E| + p^2/2m)^{-1}$ - относительно быстрозатухающей функцией, посему можно вообще положить $p = 0$. Наконец, проинтегрировав получивпееся уравнения по $(d\boldsymbol{p})$ и сократив на интеграл от волновой функции, мы получаем следующее y равиежие самосогласоважия - которое является уравнением на допустимые уровни энергии:

$$|U_{p=0}| \int \frac{(d\boldsymbol{p})}{|E| + \frac{p^2}{2m}} = 1$$

Данное уравнение устроено следующим образом.

Перед интегралом стоит Фурье-компонента потенциала, которая, в меру уравнению - сделать интеграл пропорционально большим; при этом единственный параметр, Который мы можем менять -Это энергия $|E|$; и по мере уменьшения энергии, интеграл увеличивается.

Дальнейппий анализ мы будем проводить уже Для конкретного случая пространства различной размерности.

Размерность $d = 1$ При буквально нулевой энергии, этот интеграл расходится степенным образом на малых импульсах, и сходится на больших [12] -поэтому ожидается степенная зависимость от энергии.

Подбирая достаточно маленькую энергию, можно прийти к тому, что знак равенства будет иметь место.

В действительности же, этот интеграл, разумеется, считается точно:

$$|U_{p=0}| \sqrt{\frac{m}{2|E|}} = 1 \to |E| = \frac{m}{2\hbar^2} \left| \int_{-\infty}^{\infty} U(x)dx \right|^2$$

(???????)
О случаях применений уравнения Шредингера в импульсном представлении
(пока актуальный вопрос.)
(??? пару примеров добавлю)

3.6.2 Overview of Features and Methods of Schrodinger equation

(intro to like 400 pages of this note, because there are a lot of methods and properties, so an intro will be also big)

Time-Reversal Symmetry: Basics

если сопрячь УШ, то ψ^* - тоже решение.
если $H = H*$, вообще говорят, что магнитное поле может это нарушать.
комплексно сопряжем левую задачу рассеяния.
нужно искать какую-то линейную комбинацию.

$$\psi_k^{(-)}(x) \equiv \alpha\psi_k^{(+)}(x)+\beta\left(\psi_k^{(+)}(x)\right)^* = \begin{cases} \alpha\left(e^{ikx}+re^{-ikx}\right)+\beta\left(e^{-ikx}+r^*e^{ikx}\right) \equiv t'e^{-ikx}, & x\to-\infty \\ \alpha te^{ikx}+\beta t^*e^{-ikx} \equiv e^{-ikx}+r'e^{ikx} & x\to+\infty \end{cases}$$

короче, нужно прийти к этому:

$$\begin{cases} \alpha+\beta r^* = 0 \\ \alpha r+\beta = t' \\ \alpha t \quad = r' \\ \beta t^* \quad = 1 \end{cases} \to \begin{cases} \alpha = -\frac{r^*}{t^*} \\ \beta = \frac{1}{t^*} \\ \beta = \frac{1}{t^*} \end{cases}, \quad \left[\begin{array}{l} t' = t \\ r' = -r^*t/t^* \\ r' = -r^*t/t^* \\ r' = -r^*t/t^* \end{array}\right.$$

т.о.
будем рассматривать только левую задачу рассеяния, так как в правой все такое же, только фаза сдвинута.
ну, вроде мы что-то больше можем, в самом деле.

О важности симметрий в формализме Шредингера

(я хз, зачем они нужны, тут отвечу на этот вопрос)

Качественное описание решения уравнения Шредингера (??)

(там что-то много осциллирует. пока больше не могу сказать, не знаю.)

Преобразование Галилея in Schrodinger equation (?)

Нужно сделать из $\hat{H}(t) = \frac{\hat{p}^2}{2m} + V(\hat{x}-vt)$ преобразованием новый гамильтониан:

$$\hat{H}'(t) \equiv \hat{U}(t)\hat{H}(t)\hat{U}^\dagger(t) - i\hbar\hat{U}(t)\partial_t\hat{U}^\dagger(t) = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

преобразование такое:

$$\hat{U} = e^{i(\frac{mv}{\hbar}\hat{x}+\frac{mv}{2\hbar}t)}\hat{T}_{-vt}$$

Понятно, что наша система отсчета должна сдвигаться, так что начнем с $\hat{U} = \hat{T}_{-vt} = e^{-vt\partial_x} = e^{-ivt\hat{p}/\hbar}$. $\hat{p}$ не меняется, так что это уже хорошо, посмотрим первую часть преобразованного Гамильтониана $\hat{U}V(x-vt)\hat{U}^\dagger$ по действию на волновую функцию:

$$\hat{T}_{-vt}V(x-vt)\hat{T}_{vt}|\psi\rangle(x) = \hat{T}_{-vt})V(x-vt)|\psi\rangle(x-vt)) = V(x)|\psi\rangle(x)$$

заметим, что все хорошо получилось потому что $\hat{T}_{-vt}$ по итогу сдвиг вернул назад. (важно понимать, что оператор действует на все, что справа от него стоит.)
Окей, все хорошо, но в гамильтониане $\hat{H}'$ появляется еще один член:

$$-i\hbar\hat{U}\partial_t\hat{U}^\dagger = -i\hbar v\hat{T}_{-vt}\hat{T}_{vt}\partial_x = -iv\hbar\partial_x = -v\hat{p}.$$

Так что над новым гамильтонианом нужно сделать какое-то преобразование...
Поищем его в общем виде $\hat{U}' = e^{i(\alpha\hat{x}+\beta t)}$.
Запишем уравнение для $\hat{H}'' = \hat{U}'\hat{H}'\hat{U}'^\dagger - i\hbar\hat{U}'\partial_t\hat{U}'^\dagger \equiv \hat{H}$, по итоге решение такое:

$$\hat{U}' = e^{i(\frac{mv}{\hbar}\hat{x}+\frac{mv}{2\hbar}t)}$$

Получается, что преобразование такое:

$$\hat{U} = e^{i(\frac{mv}{\hbar}\hat{x}+\frac{mv}{2\hbar}t)}\hat{T}_{-vt}$$

(???? где оно применяется????)

интегралы движения в представлении Шредингера

(киселев стр 41)
Интегралы получаются из теоремы Нетер (???)

$$\mathrm{i}\hbar\frac{d\hat{f}}{dt} = \mathrm{i}\hbar\frac{\partial\hat{f}}{\partial t} + [\hat{f},\hat{H}]$$

$$[\hat{f},\hat{H}] = 0$$

$$\frac{df}{dt} = -\frac{\partial H}{\partial\phi} = \{f,H\}_{\mathrm{P}}$$

согласно теореме Нётер, параметрическая замена

$$\frac{dS}{du} = \int dt\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{\phi}}\frac{\partial\phi'}{\partial u}\right)$$

$$\frac{\partial\phi'}{\partial u} = 1$$

$$\frac{\partial L}{\partial\dot{\phi}} = f$$

$$\frac{dS}{du} = \int dt\frac{df}{dt} = 0$$

посмотрим на два интеграла, какие есть условия вырождения? (стр 43 киселев????)

$$[\hat{f},\hat{H}] = 0, \quad [\hat{g},\hat{H}] = 0$$

$$[\hat{f},\hat{g}] = \mathrm{i}\hbar\hat{C}$$

$$\hat{H}\hat{g}|\Psi\rangle = \hat{g}\hat{H}|\Psi\rangle = E\hat{g}|\Psi\rangle$$

$$\hat{H}\hat{g}|\Psi\rangle = \hat{g}\hat{H}|\Psi\rangle = E\hat{g}|\Psi\rangle$$

$$\hat{g}|\Psi\rangle = \sum_k c_k \left|E, f_k\right\rangle, \quad |\Psi\rangle = |E, f_0\rangle$$

вывод про вырожденность.

Do we need to know mathematics of 1D Schrödinger Equation?

(currently, I don't see arguments to study it, but okay, maybe I'll understand them later and write them here)

3.6.3 Mathematics of 1D Schrödinger Equation 1

Theory

Here we describe the general properties of the Schrodinger operator for a quantum particle in $\mathbb{R}^n$ moving in a potential field. To simplify the notation, in this chapter we set $\hbar = 1$ and $m = \frac{1}{2}$, and use $\boldsymbol{x} = (x_1, ..., x_n)$ for Cartesian coordinates on $\mathbb{R}^n$. Recall (see Section 2.4 in Chapter 2) that the corresponding Schrodinger operator is given by the formal differential expression

$$H = -\Delta + V(\boldsymbol{x})$$

where $V(\boldsymbol{x})$ is a real-valued, measurable function on $\mathbb{R}^n$. Denote by

$$H_0 = -\Delta = -\left(\frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_n^2}\right)$$

the Schrodinger operator of a free quantum particle of mass $m = \frac{1}{2}$ on $\mathbb{R}^n$, also called the kinetic energy operator, and by V - the multiplication by $V(\boldsymbol{x})$ operator, also called the potential energy operator, so that

$$H = H_0 + V. \tag{1.1}$$

According to Section 2.3 of Chapter 2, the operator H_0 is self-adjoint and unbounded on $\mathscr{H} = L^2(\mathbb{R}^n)$, with the domain $D(H_0) = W^{2,2}(\mathbb{R}^n)$ and absolutely continuous spectrum $[0, \infty)$, and the operator V is self-adjoint and is bounded if and only if $V(\boldsymbol{x}) \in L^\infty(\mathbb{R}^n)$, when $\|V\| = \|V\|_\infty$. The sum $H_0 + V$ is not necessarily self-adjoint, and the first major mathematical problem of quantum mechanics is to characterize potentials $V(x)$ for which the formal differential expression (1.1) uniquely defines a self-adjoint operator H on $\mathscr{H}$. We start by presenting some useful criteria for the self-adjointness.

1.1. Self-adjointness.

The main result here is the Kato-Rellich theorem on perturbation of self-adjoint operators.

Definition. Let A and B be densely defined operators in $\mathscr{H}$. The operator B is smaller than A in the sense of Kato if $D(A) \subseteq D(B)$ and there exist $a, b \in \mathbb{R}$ with $a < 1$ such that for all $\psi \in D(A)$,

$$\|B\psi\| \leq a\|A\psi\| + b\|\psi\| \tag{1.2}$$

Equivalently, the operator B is smaller than A in the sense of Kato, if there exist $\alpha, \beta \in \mathbb{R}$ with $\alpha < 1$ such that for all $\psi \in D(A)$,

$$\|B\psi\|^2 \leq \alpha\|A\psi\|^2 + \beta\|\psi\|^2 \tag{1.3}$$

Kato-Rellich Theorem

If A is a self-adjoint operator with domain $D(A)$ and B is a symmetric operator smaller than A in the sense of Kato, then $H = A + B$ with $D(H) = D(A)$ is a self-adjoint operator.

Proof.

Recall that the operator H is self-adjoint if and only if $\mathrm{Im}(H + \lambda I) = \mathrm{Im}(H - \lambda I) = \mathscr{H}$ for some $\lambda \in i\mathbb{R}$, and hence for all $\lambda \in \mathbb{C}\backslash\sigma(H)$. Since $A = A^*$, for every $\lambda \in i\mathbb{R}$ we have $R_\lambda = (A - \lambda I)^{-1} \in \mathscr{L}(\mathscr{H})$ and $\mathrm{Im}\, R_\lambda = D(A)$. Now

$$H - \lambda I = (I + BR_\lambda)\,(A - \lambda I)$$

and in order to prove that $\mathrm{Im}(H - \lambda I) = \mathscr{H}$ it is sufficient to show that for $|\lambda|$ large enough $\|BR_\lambda\| < 1$, since then by Neumann series $I + BR_\lambda$ is an invertible bounded operator and $\mathrm{Im}\,(I + BR_\lambda) = \mathscr{H}$. Indeed, for all $\varphi \in \mathscr{H}$ we have the inequalities

$$\|R_\lambda\varphi\| \leq \frac{1}{|\lambda\|}\|\varphi\| \quad \text{and} \quad \|AR_\lambda\varphi\| \leq \|\varphi\|$$

which follow from the equation $\|(A-\lambda I)\psi\|^2 = \|A\psi\|^2 + |\lambda|^2\|\psi\|^2$ by setting $\varphi = (A-\lambda I)\psi$. Now using (1.2) with $\psi = R_\lambda\varphi$, we get

$$\|BR_\lambda\varphi\| \leq a\,\|AR_\lambda\varphi\| + b\,\|R_\lambda\varphi\| \leq \left(a + \frac{b}{|\lambda|}\right)\|\varphi\|,$$

so that $\|BR_\lambda\| < 1$ for large enough $|\lambda|$.

We use the Kato-Rellich criterion for the physically important case when $A = H_0$ - the Schrodinger operator of a free particle in $\mathbb{R}^3$ - and $B = V$ - the multiplication by $V(\boldsymbol{x})$ operator.

Theorem 1.2.

Let $V = V_1 + V_2$, where $V_1(\boldsymbol{x}) \in L^2(\mathbb{R}^3)$ and $V_2(\boldsymbol{x}) \in L^\infty(\mathbb{R}^3)$. Then $H = H_0 + V$ is a self-adjoint operator and $D(H) = W^{2,2}(\mathbb{R}^3)$.

Proof. It is sufficient to show that V is smaller than H_0 in the sense of Kato on $C_0^\infty(\mathbb{R}^3) \subset W^{2,2}(\mathbb{R}^3)$. Denoting by $\|\cdot\|_\infty$ the norm in $L^\infty(\mathbb{R}^3)$, for $\varphi \in C_0^\infty(\mathbb{R}^3)$ we have

$$\|V\varphi\| \leq \|V_1\|\,\|\varphi\|_\infty + \|V_2\|_\infty\,\|\varphi\|.$$

Let $h(\boldsymbol{p}) = \boldsymbol{p}^2$. Denoting by $\|\cdot\|_1$ the norm in $L^1(\mathbb{R}^3)$ and using the Fourier transform and the Cauchy-Bunyakovski-Schwarz inequality, we get

$$\begin{aligned}(2\pi)^{3/2}\|\varphi\|_\infty &= \sup_{\boldsymbol{x}\in\mathbb{R}^3}\left|\int_{\mathbb{R}^3} e^{i\boldsymbol{p}\boldsymbol{x}}\breve{\varphi}(\boldsymbol{p})d^3\boldsymbol{p}\right| \leq \|\breve{\varphi}\|_1 \\ &\leq \left\|(h+1)^{-1}\right\|\,\|(h+1)\breve{\varphi}\| \leq C(\|h\breve{\varphi}\| + \|\breve{\varphi}\|) \\ &= C\,(\|H_0\varphi\| + \|\varphi\|)\,.\end{aligned}$$

Now replace $\breve{\varphi}(\boldsymbol{p})$ by $\breve{\varphi}_r(\boldsymbol{p}) = r^3\breve{\varphi}(r\boldsymbol{p}), r > 0$. Since $\|\breve{\varphi}_r\|_\infty = \|\breve{\varphi}\|_\infty, \|\breve{\varphi}_r\|_1 = \|\breve{\varphi}\|_1, \|\breve{\varphi}_r\| = r^{3/2}\|\breve{\varphi}\|$, and $\|h\breve{\varphi}_r\| = r^{-1/2}\|h\breve{\varphi}\|$, we get

$$(2\pi)^{3/2}\|\varphi\|_\infty \le r^{-1/2}C\left(\|H_0\varphi\| + r^2\|\varphi\|\right)$$

where $r > 0$ is arbitrary. Choosing r such that $a = r^{-1/2}(2\pi)^{-3/2}C\,\|V_1\| < 1$ completes the proof.

Corollary 1.3. The Schrodinger operator of a complex atom, considered in Example 2.2 in Section 2.4 of Chapter 2, is essentially self-adjoint on $C_0^\infty\left(\mathbb{R}^{3(N+1)}\right)$.

Proof. We consider only the special case of the Hamiltonian of the hydrogen atom,

$$H = -\Delta - \frac{e^2}{r}, \quad r = |\boldsymbol{x}|.$$

Writing $V = \chi_1 V + (1-\chi_1)\,V = V_1 + V_2$, where χ_1 is the characteristic function of the unit ball $B_1 = \{x \in \mathbb{R}^3 : |x| \le 1\}$, we have $V_1(\boldsymbol{x}) \in L^2(\mathbb{R}^3)$ and $V_2(\boldsymbol{x}) \in L^\infty(\mathbb{R}^3)$.

Another useful criterion applies to real-valued potentials $V(\boldsymbol{x}) \in L^\infty_{\text{loc}}(\mathbb{R}^n)$, the space of locally bounded a.e. functions on $\mathbb{R}^n$. In this case the operator H, defined by the formal differential expression (1.1), is symmetric on $C_0^\infty(\mathbb{R}^n)$ and we have the following result.

Theorem 1.4. If $V(\boldsymbol{x}) \in L^\infty_{\text{loc}}(\mathbb{R}^n)$ is bounded from below, $V(\boldsymbol{x}) \ge C$ a.e. on $\mathbb{R}^n$, then the Schrodinger operator $H = H_0 + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

In fact, a much more general statement holds.

Theorem 1.5 (Sears). Suppose that the potential $V(\boldsymbol{x}) \in L^\infty_{\text{loc}}(\mathbb{R}^n)$ for all $\boldsymbol{x} \in \mathbb{R}^n$ satisfies the condition

$$V(\boldsymbol{x}) \ge -Q(|\boldsymbol{x}|),$$

where $Q(r)$ is an increasing continuous positive function on $[0,\infty)$ such that

$$\int_0^\infty \frac{dr}{\sqrt{Q(r)}} = \infty$$

Then the Schrodinger operator $H = H_0 + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

Problem 1.1. Prove the general case of Corollary 1.3 (Hint: Derive the estimate (1.3) for each term in the corresponding potential energy operator.)

Problem 1.2 (Kato's inequality). Let $\psi \in L^1_{\text{loc}}(\mathbb{R}^n)$ be such that $\Delta\psi$, defined in the distributional sense, is represented by a function in $L^1_{\text{loc}}(\mathbb{R}^n)$. Prove that in the distributional sense, $\Delta|u| \ge \operatorname{Re}\left(\frac{\overline{u}}{u}\Delta u\right)$, where it is assumed that $\frac{\overline{u(\boldsymbol{x})}}{u(\boldsymbol{x})} = 0$ if $u(\boldsymbol{x}) = 0$. (The distribution $T \in \mathscr{S}(\mathbb{R}^n)'$ is non-negative if $T(\varphi) \ge 0$ for all non-negative $\varphi \in \mathscr{S}(\mathbb{R}^n)$.)

Problem 1.3. Prove Theorem 1.4 using Kato's inequality. (Hint: Show that if $\psi \in L^2(\mathbb{R}^n)$ in the distributional sense satisfies $(-\Delta + V(\boldsymbol{x}) + C + 1)\psi = 0$, then $\psi = 0$.)

Problem 1.4. Prove that one-dimensional Schrodinger operators with unbounded below potentials $V(x) = x$ and $V(x) = -x^2$ are essentially self-adjoint on $C_0^\infty(\mathbb{R})$.

1.2. Characterization of the spectrum.

The second major mathematical problem in quantum mechanics is to describe the spectral properties of the Schrodinger operator H. Here we present some general results characterizing the spectrum of H. The first basic result is the following.

Theorem 1.6. Suppose that $V(\boldsymbol{x}) \in L^\infty_{\text{loc}}(\mathbb{R}^n)$ satisfies

$$\lim_{|x|\to\infty} V(x) = \infty$$

Then the operator H has a pure point spectrum: there exists an orthonormal basis $\{\psi_n\}_{n\in\mathbb{N}}$ for $\mathscr{H}$ consisting of eigenfunctions of H with eigenvalues $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n \le \cdots$ of finite multiplicity,

$$H\psi_n = \lambda_n \psi_n,$$

and $\lim_{n\to\infty} \lambda_n = \infty$.

Recall that the essential spectrum $\sigma_{\text{ess}}(A)$ of a self-adjoint operator A consists of all non-isolated points of $\sigma(A)$ and of eigenvalues of infinite multiplicity. The following result gives a sufficient condition for the essential spectrum of the Schrodinger operator to fill $[0,\infty)$.

Theorem 1.7. Suppose that $V = V_1 + V_2$, where $V_1(\boldsymbol{x}) \in L^q(\mathbb{R}^n), 2q \ge n$ for $n > 4$ and $q \ge 2$ for $n \le 4$[1], and $V_2(\boldsymbol{x}) \in L^\infty(\mathbb{R}^n)$ satisfies

$$\lim_{|\boldsymbol{x}|\to\infty} V_2(\boldsymbol{x}) = 0$$

Then $\sigma_{\text{ess}}(H) = [0,\infty)$, so that $\sigma(H) \cap (-\infty, 0)$ consists of isolated eigenvalues of H of finite multiplicity.

The next result gives a sufficient condition for the Schrodinger operator with decaying potential to have only negative eigenvalues.

Theorem 1.8 (Kato). Suppose that $V(\boldsymbol{x}) \in L^\infty(\mathbb{R}^n)$ and

$$\lim_{|\boldsymbol{x}|\to\infty} |\boldsymbol{x}| V(\boldsymbol{x}) = 0$$

Then the Schrodinger operator $H = H_0 + V$ has no positive eigenvalues.

Recall that the absolutely continuous spectrum and the singular spectrum of a self-adjoint operator A on $\mathscr{H}$ are defined, respectively, by $\sigma_{\text{ac}}(A) = \sigma\left(A|_{\mathscr{H}_{\text{ac}}}\right)$ and $\sigma_{\text{sc}}(A) = \sigma\left(A|_{\mathscr{H}_{\text{sc}}}\right)$, where $\mathscr{H}_{\text{ac}}$ and $\mathscr{H}_{\text{sc}}$ are closed subspaces for A defined as follows. Let P_A be the projection-valued measure for the self-adjoint operator A and let $\nu_\psi = (\mathrm{P}_A\psi, \psi)$ be the finite Borel measure on $\mathbb{R}$ corresponding to $\psi \in \mathscr{H}, \psi \ne 0$. Then $\mathscr{H}_{\text{ac}}$ consists of 0 and all $\psi \in \mathscr{H}$ such that the measure ν_ψ is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}$, and $\mathscr{H}_{\text{sc}}$ consists of 0 and all $\psi \in \mathscr{H}$ such that the measure ν_ψ is continuous singular with respect to the Lebesgue measure on $\mathbb{R}$.

Theorem 1.9. Suppose that the potential $V(\boldsymbol{x}) \in L^\infty(\mathbb{R}^n)$ for some $\varepsilon > 0$ satisfies

$$V(\boldsymbol{x}) = O\left(|\boldsymbol{x}|^{-1-\varepsilon}\right) \quad \text{as} \quad |\boldsymbol{x}| \to \infty.$$

Then the Schrodinger operator $H = H_0 + V$ has no singular spectrum and $\sigma_{\text{ac}}(H) = [0,\infty)$. Moreover, $\sigma(H) \cap (-\infty, 0)$ consists of eigenvalues of H of finite multiplicity with the only possible accumulation point at 0 .

Finally, for the physically important case $n = 3$ there is a useful estimate for the number of eigenvalues of the Schrodinger operator.

Theorem 1.10 (Birman-Schwinger). Suppose that $V(\boldsymbol{x}) \in L^\infty(\mathbb{R}^3)$ and

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|V(\boldsymbol{x})V(\boldsymbol{y})|}{|\boldsymbol{x}-\boldsymbol{y}|^2} d^3\boldsymbol{x} d^3\boldsymbol{y} < \infty.$$

Then for the total number N of eigenvalues of the Schrodinger operator $H = H_0 + V$, counted with multiplicities, we have

$$N \le \frac{1}{16\pi^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|V(\boldsymbol{x})V(\boldsymbol{y})|}{|\boldsymbol{x}-\boldsymbol{y}|^2} d^3\boldsymbol{x} d^3\boldsymbol{y}.$$

[1] In the special case $n = 4$ one has $q > 2$.

Problem 1.5. Prove all results stated in this section. (Hint: See the list of references to this chapter.)

1.3. The virial theorem.

Let $H = H_0 + V$ be the Schrodinger operator whose potential is a homogeneous function on $\mathbb{R}^n$ of degree ρ, i.e., $V(a\boldsymbol{x}) = a^\rho V(\boldsymbol{x})$. The virial theorem in quantum mechanics is the relation between the expectation values of the kinetic and potential energy operators H_0 and V in the stationary state.

Theorem 1.11 (The virial theorem). Let $\psi \in \mathscr{H}, \|\psi\| = 1$, be the eigenfunction of the Schrodinger operator with the homogeneous potential of degree ρ, and let $T_0 = (H_0\psi, \psi)$ and $V_0 = (V\psi, \psi)$ be the corresponding expectation values of kinetic and potential energy operators. Then

$$2T_0 = \rho V_0.$$

Proof. It follows from the Schrodinger equation

$$-\Delta\psi + V(\boldsymbol{x})\psi = \lambda\psi$$

that

$$T_0 + V_0 = -(\Delta\psi, \psi) + (V\psi, \psi) = \lambda.$$

For every $a > 0$ the function $\psi_a(\boldsymbol{x}) = \psi(a\boldsymbol{x})$ satisfies

$$-\Delta\psi_a + a^{\rho+2}V(\boldsymbol{x})\psi_a = a^2\lambda\psi_a$$

so that by differentiating this equation with respect to a at $a = 1$ and using Euler's homogenous function theorem, we get

$$-\Delta\dot{\psi} + V(\boldsymbol{x})\dot{\psi} = \lambda\dot{\psi} + (2\lambda - (\rho+2)V(\boldsymbol{x}))\psi \tag{1.4}$$

Since $\dot{\psi} \in D(H)$ and H is self-adjoint,

$$((H - \lambda I)\dot{\psi}, \psi) = (\dot{\psi}, (H - \lambda I)\psi) = 0$$

and we obtain from (1.4) that

$$2\lambda = (\rho + 2)V_0,$$

which completes the proof.

Remark. Since energy levels of quantum systems are related to the closed orbits of corresponding classical systems, Theorem 1.11 is the quantum analog of the classical virial theorem (see Example 1.2 in Section 1.3 of Chapter 1).

Problem 1.6 (The Raleigh-Ritz principle). Prove that λ is an eigenvalue of a self-adjoint operator H with the eigenfunction ψ if and only if ψ is a critical point of the functional $F(\varphi) = ((H - \lambda I)\varphi, \varphi)$ on $D(H)$.

Problem 1.7. Derive the virial theorem from the Raleigh-Ritz principle.

О случаях, когда УШ не работает, but QM works

(I heard about it, but I forgot about it. It is something about range of definition of operators, some mathematically exotic situation)

3.6.4 Mathematics of 1D Schrödinger Equation 2

The Schrodinger operator on the real line - the one-dimensional Schrodinger operator - has the form

$$H = -\frac{d^2}{dx^2} + V(x)$$

where the real-valued potential $V(x) \in L^1_{\text{loc}}(\mathbb{R})$, the space of locally integrable functions on $\mathbb{R}$. The corresponding eigenvalue problem

$$H\psi = \lambda\psi$$

reduces to the second order ordinary differential equation

$$-y'' + V(x)y = k^2 y, \quad -\infty < x < \infty \tag{2.1}$$

where it is convenient to set $\lambda = k^2$. In this section, we will study in detail the one-dimensional Schrodinger equation (2.1) for the case when

$$\int_{-\infty}^{\infty} (1 + |x|)|V(x)|dx < \infty. \tag{2.2}$$

Condition (2.2) is a mathematical formulation of the physical statement that the potential $V(x)$ decays as $|x| \to \infty$. It allows us to compare solutions $y(x, k)$ of the Schrodinger equation (2.1) with the solutions $e^{\pm ikx}$ of the Schrodinger equation for the free quantum particle, which corresponds to the case $V = 0$ in (2.1). All results in this section hold for the real-valued potential $V(x) \in L^1_{\text{loc}}(\mathbb{R})$ satisfying (2.2); to simplify the presentation we will additionally assume that the potential $V(x)$ in (2.2) is continuous on $\mathbb{R}$.

Способы определения стационарных состояний

(соберу их тут, this is relatively easy question)

Determining other properties of 1D one-particle systems using Schrodinger equation

О нахождении среднего (!!!)

(укажу тут что-то про это, вроде просто по обычной формуле смело считаем и все.)

Typical mathematical transformations for Schrodinger equation

(важное указание, как не тратить время на них.)

When strict mathematical transformations for Schrodinger equation are essential and when one can without problems work with basic methods?

(this is the general question, after which one will understand why he should at all read about math about Shr. eq. And this is a very important question.)

2.1. Jost functions and transition coefficients.

Let

$$\sigma(x) = \int_x^\infty |V(s)|ds \quad \text{and} \quad \sigma_1(x) = \int_x^\infty \sigma(s)ds$$

Since $V \in L^1(\mathbb{R})$, we have $\lim_{x\to\infty} \sigma(x) = 0$, and using condition (2.2) and the Fubini theorem we get
$\sigma_1(x) = \int_x^\infty \int_s^\infty |V(t)|dtds = \int_x^\infty \int_x^t |V(t)|dsdt = \int_x^\infty (t-x)|V(t)|dt < \infty$, so that $\sigma \in L^1(x,\infty)$ for all $x \in \mathbb{R}$ and $\lim_{x\to\infty} \sigma_1(x) = 0$. Similarly, the functions

$$\tilde\sigma(x) = \int_{-\infty}^x |V(s)|ds \quad \text{and} \quad \tilde\sigma_1(x) = \int_{-\infty}^x \tilde\sigma(s)ds$$

satisfy $\lim_{x\to-\infty} \tilde\sigma(x) = \lim_{x\to-\infty} \tilde\sigma_1(x) = 0$. Condition (2.2) ensures that for real k the differential equation (2.1) has solutions $f_1(x,k)$ and $f_2(x,k)$,
uniquely defined by the following asymptotics:

$$f_1(x,k) = e^{ikx} + o(1) \quad \text{as} \quad x \to \infty$$
$$f_2(x,k) = e^{-ikx} + o(1) \quad \text{as} \quad x \to -\infty$$

They are called Jost solutions and play a fundamental role in the theory of a one-dimensional Schrodinger equation.

Theorem 2.1. For real k the differential equation (2.1) has solutions $f_1(x,k)$ and $f_2(x,k)$ satisfying the following properties.
(i) Estimates for $k \in \mathbb{R}$:

$$\left|e^{-ikx} f_1(x,k) - 1\right| \le \left(\sigma_1(x) - \sigma_1\left(x + \frac{1}{|k|}\right)\right) e^{\sigma_1(x)}$$
$$\left|e^{ikx} f_2(x,k) - 1\right| \le \left(\tilde\sigma_1(x) - \tilde\sigma_1\left(x - \frac{1}{|k|}\right)\right) e^{\tilde\sigma_1(x)}$$

(ii) Asymptotics as $|x| \to \infty$:

$$\lim_{x\to\infty} e^{-ikx} f_1(x,k) = 1, \lim_{x\to\infty} e^{-ikx} f_1'(x,k) = ik$$
$$\lim_{x\to-\infty} e^{ikx} f_2(x,k) = 1, \lim_{x\to-\infty} e^{ikx} f_1'(x,k) = -ik$$

(iii) Analyticity: $f_1(x,k)$ and $f_2(x,k)$ admit analytic continuation to the upper half-plane $\operatorname{Im} k > 0$, and are continuous functions on $\operatorname{Im} k \ge 0$, uniformly in x on compact subsets of $\mathbb{R}$.
(iv) The conjugation property:

$$\overline{f_1(x,k)} = f_1(x,-\bar k), \quad \overline{f_2(x,k)} = f_2(x,-\bar k), \quad \operatorname{Im} k \ge 0$$

(v) Estimates in part (i) hold for $\operatorname{Im} k \ge 0$. For $k \ne 0$,

$$\left|f_1(x,k) - e^{ikx}\right| \le \frac{e^{-\operatorname{Im} kx}}{|k|}\sigma(x)e^{\frac{1}{|k|}\sigma(x)}$$
$$\left|f_2(x,k) - e^{-ikx}\right| \le \frac{e^{\operatorname{Im} kx}}{|k|}\tilde\sigma(x)e^{\frac{1}{|k|}\tilde\sigma(x)}$$

(vi) Asymptotics as $|k| \to \infty, \operatorname{Im} k \ge 0$:

$$e^{-ikx} f_1(x,k) = 1 + O\left(|k|^{-1}\right), \quad e^{ikx} f_2(x,k) = 1 + O\left(|k|^{-1}\right)$$

Proof. It follows from the method of variation of parameters that differential equation (2.1) with the boundary condition $\lim_{x\to\infty} e^{-ikx} f_1(x,k) = 1$ is equivalent to the integral equation

$$f_1(x,k) = e^{ikx} - \int_x^\infty \frac{\sin k(x-t)}{k} V(t) f_1(t,k)\,dt \tag{2.3}$$

Setting $\varphi(x,k) = e^{-ikx} f_1(x,k)$, we get

$$\varphi(x,k) = 1 - \int_x^\infty \frac{1 - e^{-2ik(x-t)}}{2ik} V(t)\varphi(t,k)\,dt. \tag{2.4}$$

For $\operatorname{Im} k \geq 0$ the integral equation (2.4) is of Volterra type and can be solved by the method of successive approximations. Namely, we look for the solution in the form

$$\varphi(x,k) = \sum_{n=0}^{\infty} \varphi_n(x,k) \tag{2.5}$$

where $\varphi_0(x,k) = 1$ and

$$\begin{aligned}\varphi_{n+1}(x,k) &= -\int_x^\infty \frac{1 - e^{-2ik(x-t)}}{2ik} V(t)\varphi_n(t,k)\,dt \\ &= \int_x^\infty \left(\int_x^t e^{-2ik(x-s)} V(t)\varphi_n(t,k)\,ds \right) dt\end{aligned}$$

From here we conclude that for $\operatorname{Im} k \geq 0$

$$|\varphi_n(x,k)| \leq \frac{\sigma_1(x)^n}{n!}. \tag{2.6}$$

Indeed, this estimate is true for $n = 0$, and using the Fubini theorem and the induction hypothesis we get

$$\begin{aligned}|\varphi_{n+1}(x,k)| &\leq \frac{1}{n!} \int_x^\infty \left(\int_x^t |V(t)| \sigma_1(t)^n ds \right) dt \\ &= \frac{1}{n!} \int_x^\infty \left(\int_s^\infty |V(t)| \sigma_1(t)^n dt \right) ds \\ &\leq \frac{1}{n!} \int_x^\infty \sigma(s) \sigma_1(s)^n ds = \frac{\sigma_1(x)^{n+1}}{(n+1)!}\end{aligned}$$

Thus

$$|\varphi(x,k)| \leq e^{\sigma_1(x)}. \tag{2.7}$$

By the Weierstrass M-test the function $\varphi(x,k)$, defined by convergent series (2.5), is analytic for $\operatorname{Im} k > 0$. It is also continuous up to $\operatorname{Im} k = 0$ uniformly in x on compact subsets of $\mathbb{R}$.

The first estimate in part (i) now follows from (2.4) and (2.7). Namely, using $|V(t)| = -\sigma'(t)$ and integration by parts, we obtain

$$\begin{aligned}|\varphi(x,k) - 1| &\leq \int_x^\infty \left| \frac{1 - e^{-2ik(x-t)}}{2ik} \right| |V(t)| |\varphi(t,k)|\,dt \\ &\leq e^{\sigma_1(x)} \left(\int_x^{x+\frac{1}{|k|}} (t-x)|V(t)|\,dt + \frac{1}{|k|} \int_{x+\frac{1}{|k|}}^\infty |V(t)|\,dt \right) \\ &= e^{\sigma_1(x)} \left(-(t-x)\sigma(t)\Big|_x^{x+\frac{1}{|k|}} + \int_x^{x+\frac{1}{|k|}} \sigma(t)\,dt + \frac{1}{|k|} \int_{x+\frac{1}{|k|}}^\infty |V(t)|\,dt \right) \\ &= e^{\sigma_1(x)} \left(\sigma_1(x) - \sigma_1\left(x + \frac{1}{|k|} \right) \right).\end{aligned}$$

For $k = 0$ this estimate should be understood as $|\varphi(x,0) - 1| \le \sigma_1(x) e^{\sigma_1(x)}$. The function $f_1(x,k) = e^{ikx}\varphi(x,k)$ satisfies the integral equation (2.3), and (2.7) allows us to differentiate under the integral sign in (2.3). This proves that $f_1(x,k)$ satisfies the differential equation (2.1) and the first estimate in part (i). In particular, $\lim_{x\to\infty} e^{-ikx} f_1(x,k) = 1$ for $\operatorname{Im} k \ge 0$. Differentiating (2.3) and using $e^{-\operatorname{Im} k(t-x)} |\cos k(x-t)| \le 1$ for $t \ge x$ and $\operatorname{Im} k \ge 0$, we obtain

$$\left| e^{-ikx} f_1'(x,k) - ik \right| \le \int_x^\infty |V(t)| |\varphi(t,k)| dt \le \sigma(x) e^{\sigma_1(x)} \tag{2.8}$$

so that $\lim_{x\to\infty} e^{-ikx} f_1'(x,k) = ik$ for $\operatorname{Im} k \ge 0$.

The conjugation property follows from the uniqueness of the solution $f_1(x,k)$ satisfying the estimate in part (i). To prove the uniqueness, denote by $\chi(x,k)$ the homogeneous solution of the integral equation (2.4) with the property that $\alpha(x) = \sup_{x \le t < \infty} |\chi(t,k)| < \infty$ for all $x \in \mathbb{R}$. Consider the inequality

$$|\chi(x,k)| \le \int_x^\infty \left(\int_x^t |V(t)| |\chi(t,k)| ds \right) dt$$

which follows from the homogeneous form of equation (2.4). Repeating the proof of the estimate (2.6), we get $|\chi(x,k)| \le \alpha(x) \frac{\sigma_1(x)^n}{n!}$, and passing to the limit $n \to \infty$ gives $\chi(x,k) = 0$.

To prove the first estimate in part (v), consider the inequality

$$|\varphi(x,k) - 1| \le \frac{\sigma(x)}{|k|} - \frac{1}{|k|} \int_x^\infty \sigma'(t) |\varphi(t,k) - 1| dt \tag{2.9}$$

which follows from (2.4) for $k \ne 0$. Iterating (2.9) we get

$$|\varphi(x,k) - 1| \le \frac{\sigma(x)}{|k|} e^{\frac{1}{|k|}\sigma(x)}$$

The asymptotic in part (vi) follows from the estimate in part (v), which completes the proof for the solution $f_1(x,k)$. The existence and analytic properties of the solution $f_2(x,k)$ are proved similarly by considering the integral equation

$$f_2(x,k) = e^{-ikx} + \int_{-\infty}^x \frac{\sin k(x-t)}{k} V(t) f_2(t,k) dt \tag{2.10}$$

Corollary 2.2. For $\operatorname{Im} k \ge 0$ and $k \ne 0$,
$\lim_{x\to\infty} e^{-ikx} \left(\dot f_1(x,k) - ix f_1(x,k) \right) = 0$, $\quad \lim_{x\to-\infty} e^{ikx} \left(\dot f_2(x,k) + ix f_2(x,k) \right) = 0$, where the dot stands for the partial derivative with respect to k.

Proof. Differentiating (2.4) with respect to k we obtain the following integral equation for $\dot\varphi(x,k) = e^{-ikx} \left(\dot f_1(x,k) - ix f_1(x,k) \right)$:

$$\dot\varphi(x,k) = g(x,k) - \int_x^\infty \frac{1 - e^{-2ik(x-t)}}{2ik} V(t) \dot\varphi(t,k) dt,$$

where

$$g(x,k) = \frac{1}{k} \int_x^\infty (t-x) e^{-2ik(x-t)} V(t) \varphi(t,k) dt + \frac{1}{k}(1 - \varphi(x,k)).$$

It follows the estimate in part (i) of Theorem 2.1 and (2.7) that $|g(x,k)| \le \frac{2}{|k|} \sigma_1(x) e^{\sigma_1(x)}$, and repeating the proof of the estimate (2.7), we obtain that $|\dot\varphi(x,k)| \le \frac{2}{|k|} \sigma_1(x) e^{2\sigma_1(x)}$. Since $\lim_{x\to\infty} \sigma_1(x) = 0$, this proves the statement for $f_1(x,k)$. The corresponding result for $f_2(x,k)$ is proved similarly.

For real $k \neq 0$ the pairs $f_1(x,k), f_1(x,-k) = \overline{f_1(x,k)}$ and $f_2(x,k),\ f_2(x,-k) = \overline{f_2(x,k)}$ are fundamental solutions of the differential equation (2.1). Indeed, the Wronskian $W(y_1,y_2) = y_1'y_2 - y_1y_2'$ of two solutions of (2.1) does not depend on x, and we get from part (ii) that

$$W(f_1(x,k), f_1(x,-k)) = \lim_{x\to\infty} W(f_1(x,k), f_1(x,-k)) = 2ik,$$
$$W(f_2(x,k), f_2(x,-k)) = \lim_{x\to-\infty} W(f_2(x,k), f_2(x,-k)) = -2ik.$$

Therefore for such k we have

$$f_2(x,k) = a(k)f_1(x,-k) + b(k)f_1(x,k) \tag{2.11}$$

where the transition coefficients $a(k)$ and $b(k)$ are given by
(2.12) $a(k) = \frac{1}{2ik}W(f_1(x,k), f_2(x,k)), \quad b(k) = \frac{1}{2ik}W(f_2(x,k), f_1(x,-k))$, and satisfy $\overline{a(k)} = a(-k), \overline{b(k)} = b(-k)$. Similarly we find that

$$f_1(x,k) = a(k)f_2(x,-k) - b(-k)f_2(x,k) \tag{2.13}$$

Back substituting (2.13) for $f_1(x,k)$ and $f_1(x,-k)$ into (2.11), for real $k \neq 0$ we find the so-called normalization condition,

$$|a(k)|^2 = 1 + |b(k)|^2. \tag{2.14}$$

It follows from parts (iii) and (vi) of Theorem 2.1 that coefficient $a(k)$ admits analytic continuation to $\operatorname{Im} k > 0$ and

$$a(k) = 1 + O\left(|k|^{-1}\right) \quad \text{as} \quad |k| \to \infty \tag{2.15}$$

Moreover, the function $ka(k)$ is continuous in $\operatorname{Im} k \geq 0$.
Normalization condition (2.14) implies that all zeros of $a(k)$ are in the upper half-plane $\operatorname{Im} k > 0$. Let k_0 be such a zero, $a(k_0) = 0$. It follows from the first equation in (2.12) that $W(f_1(x,k_0), f_2(x,k_0)) = 0$, so that the Jost solutions $f_1(x,k_0), f_2(x,k_0)$ are linearly dependent,

$$f_1(x,k_0) = c_0 f_2(x,k_0)$$

for some $c_0 \neq 0$. It follows from part (i) of Theorem 2.1 that for $\operatorname{Im} k > 0$ the solution $f_1(x,k)$ is exponentially decaying as $x \to \infty$, and the solution $f_2(x,k)$ is exponentially decaying as $x \to -\infty$. Therefore $f_1(\cdot,k_0) \in L^2(\mathbb{R})$ is an eigenfunction of the Schrodinger operator H with the eigenvalue $\lambda_0 = k_0^2$. Since H is symmetric, its eigenvalues are real:

$$\lambda_0 \|f_1(\cdot,k_0)\|^2 = \int_{-\infty}^{\infty} (-f_1''(x,k_0) + V(x)f_1(x,k_0))\,\overline{f_1(x,k_0)}dx$$
$$= \int_{-\infty}^{\infty} f_1(x,k_0)\left(-\overline{f_1''(x,k_0)} + V(x)\overline{f_1(x,k_0)}\right)dx = \bar{\lambda}_0 \|f_1(\cdot,k_0)\|^2$$

as is easily seen by integrating by parts twice; due to part (i) of Theorem 2.1 and estimate (2.8) the boundary terms vanish as $|x| \to \infty$. Thus $k_0 = i\varkappa_0$ is pure imaginary with $\varkappa_0 > 0$ so that $\lambda_0 = -\varkappa_0^2 < 0$, and the corresponding eigenfunction $f_1(x, i\varkappa_0)$ is real-valued.

Proposition 2.1.

The function $a(k)$ in the upper half-plane $\operatorname{Im} k > 0$ has only finitely many pure imaginary simple zeros $k_l = i\varkappa_l$, and

$$\dot{a}(i\varkappa_l) = -ic_l \|f_2(\cdot, i\varkappa_l)\|^2, \quad l = 1, ..., n$$

where the dot stands for the derivative and $f_1(x, i\varkappa_l) = c_l f_2(x, i\varkappa_l)$. The function $1/a(k)$ is bounded in some neighborhood of $k = 0$ in $\operatorname{Im} k \geq 0$.

Proof. It follows from (2.14) and (2.15) that $k = 0$ is the only possible accumulation point of zeros of $a(k)$ in $\operatorname{Im} k \geq 0$. First suppose that functions $f_1(x, k)$ and $f_2(x, k)$ are linearly independent for $k = 0$. Then the continuous in $\operatorname{Im} k > 0$ function $ka(k)$ satisfies $\lim_{k\to 0} ka(k) = W(f_1(x, 0), f_2(x, 0)) \neq 0$. Therefore $a(k) \neq 0$ in some neighborhood of 0, and $a(k)$ has only finitely many zeros in $\operatorname{Im} k > 0$.

The case when $f_1(x, 0) = cf_2(x, 0), c \neq 0$, is more subtle. Suppose that there is a converging to 0 subsequence $k_n = i\varkappa_n$ of zeros of $a(k)$ in $\operatorname{Im} k > 0$. It follows from part (i) of Theorem 2.1 that there exists $A > 0$ such that for all $\varkappa \geq 0$ we have $f_1(x, i\varkappa) > \frac{1}{2}e^{-\varkappa x}$ for $x \geq A$ and $f_2(x, i\varkappa) > \frac{1}{2}e^{\varkappa x}$ for $x \leq A$, so that

$$\int_A^\infty f_1(x, i\varkappa_n) f_1(x, 0)dx, \int_{-\infty}^{-A} f_2(x, i\varkappa_n) f_2(x, 0)dx \geq \frac{1}{4\varkappa} e^{-\varkappa A}$$

Using integration by parts, we get, as before,

$$\begin{aligned}\varkappa_n^2 \int_{-\infty}^\infty f_1(x, i\varkappa_n) f_1(x, 0)dx &= \int_{-\infty}^\infty (f_1''(x, i\varkappa_n) - V(x) f_1(x, i\varkappa_n)) f_1(x, 0)dx \\ &= \int_{-\infty}^\infty f_1(x, i\varkappa_n) (f_1''(x, 0) - V(x) f_1(x, 0))\, dx = 0\end{aligned}$$

On other hand, we have

$$\begin{aligned}0 = &\int_A^\infty f_1(x, i\varkappa_n) f_1(x, 0)dx + \int_{-A}^A f_1(x, i\varkappa_n) f_1(x, 0)dx \\ &+ c \cdot c_n \int_{-\infty}^{-A} f_2(x, i\varkappa_n) f_2(x, 0)dx\end{aligned} \tag{2.16}$$

Since $f_1(x, k)$ is continuous on $\operatorname{Im} k \geq 0$, uniformly in x on the compact subsets of $\mathbb{R}$, we have

$$\lim_{n\to\infty} \int_{-A}^A f_1(x, i\varkappa_n) f_1(x, 0)dx = \int_{-A}^A f_1(x, 0)^2 dx \geq 0$$

Using

$$\lim_{n\to\infty} c \cdot c_n = c \lim_{n\to\infty} \frac{f_1(x, i\varkappa_n)}{f_2(x, i\varkappa_n)} = c\frac{f_1(x, 0)}{f_2(x, 0)} = c^2 > 0$$

we obtain from (2.16) that for large enough n,

$$0 > \frac{1}{4\varkappa_n} e^{-\varkappa_n A}.$$

This is clearly a contradiction, so $a(k)$ has only finitely many zeros. The proof of local boundness of $1/a(k)$ in this case is left to the reader.

Next, consider the differential equation (2.1) together with the equation obtained from it by differentiating with respect to k:

$$-y'' + V(x)y = k^2 y \tag{2.17}$$
$$-\dot{y}'' + V(x)\dot{y} = k^2\dot{y} + 2ky \tag{2.18}$$

Set $y = f_1(x,k)$ in equation (2.17), $y = f_2(x,k)$ in equation (2.18), and multiply (2.17) by $\dot{f}_2(x,k)$ and (2.18) by $f_1(x,k)$. Subtracting the resulting equations, we obtain

$$W\left(f_1(x,k), \dot{f}_2(x,k)\right)' = 2kf_1(x,k)f_2(x,k)$$

Similarly, setting $y = f_2(x,k)$ in (2.17), $y = f_1(x,k)$ in (2.18), cross multiplying and subtracting, we obtain

$$-W\left(\dot{f}_1(x,k), f_2(x,k)\right)' = 2kf_1(x,k)f_2(x,k)$$

Therefore

$$W\left(f_1(x,k), \dot{f}_2(x,k)\right)\Big|_{-A}^{x} = 2k\int_{-A}^{x} f_1(x,k)f_2(x,k)dx \tag{2.19}$$
$$-W\left(\dot{f}_1(x,k), f_2(x,k)\right)\Big|_{x}^{A} = 2k\int_{x}^{A} f_1(x,k)f_2(x,k)dx \tag{2.20}$$

Now suppose that $a(k_0) = 0$. We have

$$W(f_1(x,k), f_2(x,k)) = 2ika(k),$$

so that differentiating with respect to k and setting $k = k_0$ gives

$$W\left(\dot{f}_1(x,k_0), f_2(x,k_0)\right) + W\left(f_1(x,k_0), \dot{f}_2(x,k_0)\right) = 2ik_0\dot{a}(k_0).$$

Since $f_1(x,k_0) = c_0 f_2(x,k_0)$, it follows from Theorem 2.1 and Corollary 2.2 that boundary terms in (2.19)-(2.20) vanish as $A \to \infty$, and we obtain, using that $f(x,k_0)$ is real-valued:

$$\dot{a}(k_0) = -i\int_{-\infty}^{\infty} f_1(x,k_0) f_2(x,k_0)\,dx = -ic_0\|f_2(\cdot,k_0)\|^2.$$

The eigenvalues of the Schrodinger operator H are simple. Indeed, the function $f_1(x,i\varkappa)$ is a solution of the differential equation (2.1) for $\lambda = -\varkappa^2 < 0$, which decays exponentially as $x \to \infty$. Since the Wronskian of any two solutions of (2.1) is constant, the second solution of (2.1), linearly independent with $f_1(x,i\varkappa)$, is exponentially increasing as $x \to \infty$. Thus every exponentially decaying as $x \to \infty$ solution of (2.1) for $\lambda = -\varkappa^2$ is a constant multiple of $f_1(x,i\varkappa)$. In particular, this proves that the point spectrum of H is simple. This result also follows from the simplicity of zeros of the function $a(k)$ and the eigenfunction expansion theorem, proved in the next section.

Problem 2.1 (The oscillation theorem). Let $\lambda_1 = -\varkappa_1^2 < \cdots < \lambda_n = \varkappa_n^2 < 0$ be the eigenvalues of the one-dimensional Schrodinger operator H. Prove that corresponding eigenfunctions $f_1(x,i\varkappa_l)$ have exactly $l-1$ simple zeros, $l = 1,...,n$.

Problem 2.2. Prove that for $\operatorname{Im} k \geq 0$ the Jost solution $f_1(x,k)$ admits the representation

$$f_1(x,k) = e^{ikx} + \int_x^{\infty} K_1(x,t)e^{ikt}dt$$

where

$$K(x,x)=\frac{1}{2}\int_x^\infty V(t)dt \quad \text{and} \quad |K_1(x,t)|\le\frac{1}{2}\sigma\left(\frac{x+t}{2}\right)e^{\sigma_1(x)-\sigma_1\left(\frac{x+t}{2}\right)}.$$

Moreover, the kernel $K_1(x,t)$ is differentiable and

$$\left|\frac{\partial K_1}{\partial x}(x,t)+\frac{1}{4}V\left(\frac{x+t}{2}\right)\right|\le\frac{1}{2}\sigma_1(x)\sigma\left(\frac{x+t}{2}\right)e^{\sigma_1(x)},$$

with the similar inequality for $\frac{\partial K_1}{\partial t}(x,t)$. Correspondingly, for $\operatorname{Im} k\le 0$ the Jost solution $f_2(x,k)$ admits the integral representation

$$f_2(x,k)=e^{-ikx}+\int_{-\infty}^x K_2(x,t)e^{-ikt}dt$$

where the kernel $K_2(x,t)$ satisfies similar estimates. (Hint: Show that (2.3) is equivalent to the integral equation

$$K_1(x,t)=\frac{1}{2}\int_{\frac{x+t}{2}}^\infty V(s)ds+\frac{1}{2}\int_x^\infty V(s)\int_{t-(s-x)}^{t+(s-x)}K_1(s,u)duds$$

with the condition $K_1(x,t)=0$ for $t<x$, which is solved by the method of successive approximations.)

Problem 2.3. Show that transition coefficients $a(k)$ and $b(k)$ have the representations

$$a(k)=1-\frac{1}{2ik}\int_{-\infty}^\infty V(x)dx-\frac{1}{2ik}\int_0^\infty A(t)e^{ikt}dt,\quad b(k)=\frac{1}{2ik}\int_{-\infty}^\infty B(t)e^{-ikt}dt,$$

where $A(t)\in L^1(0,\infty)$ and $B(t)\in L^1(-\infty,\infty)$.

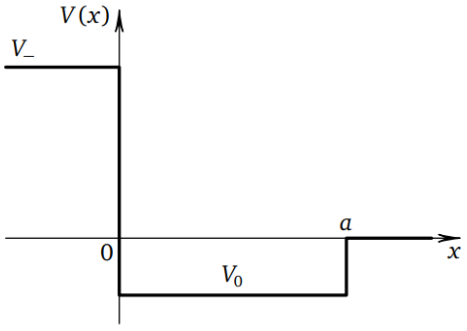
Problem 2.4. Show that for $\operatorname{Im} k>0$ the transition coefficient $a(k)$ satisfies the dispersion relation

$$a(k)=\exp\left\{\frac{1}{2\pi i}\int_{-\infty}^\infty\frac{\log\left(1+|b(p)|^2\right)}{p-k}dp\right\}\prod_{l=1}^n\frac{k-i\varkappa_l}{k+i\varkappa_l}.$$

3.6.5 1D Schrödinger Equation 2: Advanced Methods

Резонансы при одномерном движении по Киселеву (?!!????)

(из киселева стр 68)



Рассмотрим непрерывный спектр невырожденных уровней энергии в потенциале

$$V(x) = \begin{cases} V_- \to +\infty, & x < 0 \\ V_0 < 0, & 0 < x < a \\ V_+ = 0, & x > a \end{cases}$$

показанном на рис. 2.2.

По условию задачи

$$V_+ < E < V_-$$

Интервал значений координаты естественным образом разбивается на три области.

I) $x < 0$. Согласно общему рассмотрению в (5.5) решение уравнения Шрёдингера затухает на бесконечности экспоненциально, причем коэффициент затухания стремится к бесконечности:

$$x_-^2 = \frac{2m}{\hbar^2}(V_- - E) \to +\infty$$

так что при наличии в некотором интервале конечной ширины бесконечно высокого потенциала волновая функция обращается внутри этого интервала в тождественный нуль:

$$\psi_I(x) = 0, \quad x < 0$$

II) $0 < x < a$. Решение осциллирует, но поскольку по непрерывн ости волновой функции

$$\psi(0) = 0$$

решение уравнения можно выбрать с точностью до множителя вещественным, так что с учетом наличия узла в нуле

$$\psi_{II}(x) = A\sin(k_0 x), \quad \frac{\hbar^2}{2m}k_0^2 = V_0 + E$$

где связь k_0 с энергией следует из уравн ения Шредингера.

III) $x > a$. Запишем решение в виде

$$\psi_{III}(x) = e^{-\mathrm{i}kx} + Re^{\mathrm{i}kx}, \quad \frac{\hbar^2}{2m}k^2 = E$$

где первый вклад отвечает падающей из бесконечности на потенциальную яму волне, а Второй -отраженной от стенки волне.

Поскольку поток прошедшей волны равен в этой Задаче нулю, коэффициент отражения равен единице и

$$|R| = 1 \quad \to \quad R = e^{\mathrm{i}\phi}$$

Т.е. отраженная волна приобретает Дополнительную фазу рассеяния ϕ.

Для получения связи неизвестных параметров в волновой функции необходимо потребовать непрерывн ости волновой функции и ее производной в точке сшивки решений

$$\psi_{II}(a) = \psi_{III}(a), \quad \psi'_{II}(a) = \psi'_{III}(a)$$

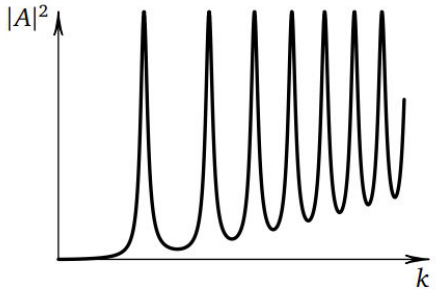
Отсюда

$$\begin{cases} A\sin(k_0 a) = \mathrm{e}^{-\mathrm{i}ka} + \mathrm{e}^{\mathrm{i}(ka+\phi)}, \\ k_0 A\cos(k_0 a) = -\mathrm{i}k\mathrm{e}^{-\mathrm{i}ka} + \mathrm{i}k\mathrm{e}^{\mathrm{i}(ka+\phi)} \end{cases} \quad \Rightarrow \quad \begin{cases} A = -2\mathrm{i}k\frac{\mathrm{e}^{-\mathrm{i}ka}}{k_0\cos(k_0 a) - \mathrm{i}k\sin(k_0 a)}, \\ \mathrm{e}^{\mathrm{i}\phi} = -\mathrm{e}^{-2\mathrm{i}ka}\frac{k_0\cos(k_0 a) + \mathrm{i}k\sin(k_0 a)}{k_0\cos(k_0 a) - \mathrm{i}k\sin(k_0 a)}. \end{cases}$$

Модуль амплитуды A, которая определяет плотность вероятности нахождения частицы в ПОТенциальной яме, задается величиной

$$|A|^2 = \frac{4k^2}{k^2 + (k_0^2 - k^2)\cos^2(k_0 a)} = \frac{4k^2}{k^2 + \frac{2m}{\hbar^2} V_0 \cos^2(k_0 a)}$$

Как видим, Квадрат модуля осциллирует в границах $0 \leqslant |A|^2 \leqslant 4$. Характерный график этой функции в зависимости от волнового вектора показан на рис. 2.3.



Пик и распределения расположены при

$$k_0 a = \frac{\pi}{2} + \pi n, \quad n \in \mathbb{N}$$

Эти пики сглаживаются, если их амплитуда мала, т.е. при

$$k^2 \gg \frac{2mV_0}{\hbar^2}$$

При обратном же соотношении пики хорошо разделены и ярко выражены.

Это имеет место при

$$k^2 \ll k_0^2 \quad \leftrightarrow \quad v \ll v_0$$

где v и v_0 -скорости дВижения волны при $x > a$ и в потенциальной яме.

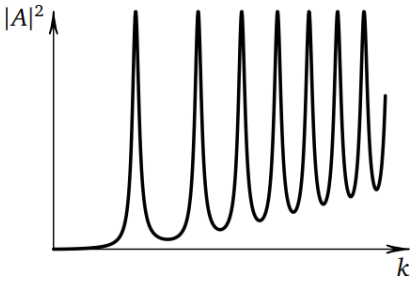


Рис. 5. Нормировка плотности вероятности обнаружить частицу в потенциальной яме в зависимости от волнового вектора падающей волны (в единицах $a = 10, -2mV_0/\hbar^2 = 200$)

Другими словами, при наличии пиков потенциальная яма выглядит глубокой для рассеивающейся частицы. С ростом энергии, естественно, потенциальная яма будет восприниматься как мелкая.

(????????)

Совершенно аналогично фаза

$$\phi = -\pi - 2ka + 2 \arctan \left[\frac{k}{k_0} \tan(k_0 a)\right]$$

вблизи пика и спытывает существенное изменение.

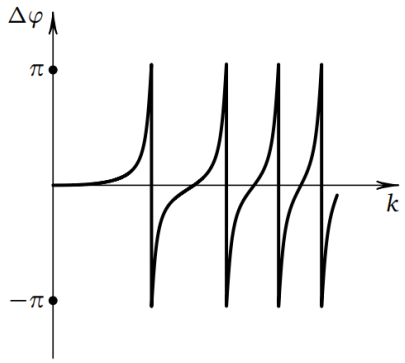
В качестве более объективной характери стики обычно рассматривают разность фаз падающей и отраженной волны, например, на границе потенциальной ямы, т.е. при $x = a$

$$\Delta\phi = 2 \arctan \left[\frac{k}{k_0} \tan(k_0 a)\right] - \pi$$

Это же значение комплексной фазы получается при умножении найденного нам и решения на фактор $\exp(\mathrm{i}2ka)$, т.е. при переопределении глобальной, не наблюдаем ой фазы волновой функции в целом.

Deeper understanding of resonances in scattering of a wall near well

Говорят, что пики амплитуды и быстрая смена фазы отвечают возбуждению резонансов в глубокой потенциальной яме. График разности фаз представлен на рис. 6, откуда видно, что вблизи пика комплексная фаза быстро меняется на 2π. Соотношение (5.45) показывает, что резонанс имеет место при условии, что в яме укладывается нечетное число четверть-волн, что в случае ямы с бесконечными стенками, т. е. потенциального ящика, соответствовало бы положению ровно посредине между стационарными уровнями энергии.



Групповая скорость волны определялась из условия стаци онарности фазы

$$\frac{\partial\phi(x,t)}{\partial p} = 0$$

так что для отраженной волны с учетом переопределения фазы, как это было сделано при выводе $\Delta\phi$

$$\phi(x,t) = px - Et + \hbar\phi, \quad p = \hbar k$$

Н

$$x = \frac{\partial E}{\partial p} t - \frac{\partial \phi}{\partial k}$$

Что можно переписать в виде

$$x = v_{\mathrm{gr}}(t - \Delta t)$$

где запаздывание по времени определим по разности фаз $\Delta\phi$

$$\Delta t = \frac{\partial\Delta\phi/\partial k}{\partial E/\partial p} = \hbar\frac{\partial\Delta\phi}{\partial E}$$

В явном виде в рассматриваемой задаче производная

$$\frac{\partial\Delta\phi}{\partial k} = \frac{2}{k^2\tan^2(k_0a)+k_0^2}\left\{\frac{ak^2}{\cos^2(k_0a)}|\frac{k_0^2-k^2}{k_0}\tan(k_0a)\right\}$$

В пике имеет значение

$$\left.\frac{\partial\Delta\phi}{\partial k}\right|_{\text{peak}} \to 2a$$

а между пиками при $\sin(k_0a)=0$

$$\frac{\partial\Delta\phi}{\partial k} \simeq 2a\frac{k^2}{k_0^2} \ll 2a$$

Эти соотношения можно проинтерпретировать следующим образом.

В классике частица проходит от одного конца ям ы до другого за время

$$\Delta t_{\text{class.}} = \frac{2a}{v_0} = m\frac{2a}{\hbar k_0}.$$

В пике, когда частицу с высокой вероятностью можно обнаружить в глубокой потенциаль- н ой яме, в квантовом случае получаем

$$\Delta t_{\text{quant.}} = m\frac{2a}{\hbar k} = m\frac{2a}{\hbar k_0}\frac{k_0}{k} \gg \Delta t_{\text{class.}}$$

Величину $\tau = \Delta t_{\text{quant.}}/4$ называют временем жизни резонанса в глубокой потенциальной ям e^4. Вне резонанса время пребывания частицы в яме даже меньше, чем в классике.

Поведение амплитуды резонанса вблизи пика

Рассмотрим поведение амплитуды резонанса вблизи пика с $k_\star \neq 0$. При этом

$$|\sin(k_0a)| \to 1, \quad \cos(k_0a) \to 0$$

так что, вводя малый параметр разложения Δk

$$k = k_\star + \Delta k, \quad \Delta k \to 0$$

находим

$$k_0 = \sqrt{\frac{2mV_0}{\hbar^2}+k^2} \to \sqrt{\frac{2mV_0}{\hbar^2}+k_\star^2+2k_\star\Delta k} \to k_0^\star + \frac{k_\star}{k_0^\star}\Delta k$$

где $k_0^\star = k_0(k_\star)$. Поскольку в пике

$$\cos(k_0^\star a) = 0, \quad k_0^\star a = \frac{\pi}{2}+\pi n$$

В окрестности пика получим

$$k_0\cos(k_0a) \to (-1)^{n+1}k_0^\star\sin\left(\frac{k_\star}{k_0^\star}a\Delta k\right) \to (-1)^{n+1}k_\star a\Delta k$$

Тогда согласно выражению для амплитуды (5.21) вблизи пика резонанса

$$A \approx -2\mathrm{i}k_\star \frac{e^{-\mathrm{i}k_\star a}}{k_0 \cos(k_0 x) - \mathrm{i}k \sin(k_0 x)} \sim \frac{1}{(-1)^{n+1} k_\star a \Delta k - (-1)^n \mathrm{i}k_\star}$$

где мы учли, что $\sin(k_0^\star a) = (-1)^n$. Выразим Δk через разн ость энергий

$$E - E_\star = \frac{\hbar^2}{2m}\left(k^2 - k_\star^2\right) = \frac{\hbar^2}{2m}(k + k_\star)\Delta k \approx \frac{\hbar^2}{m} k_\star \Delta k$$

Откуда:

$$A \sim \frac{1}{\frac{ma}{\hbar^2}(E - E_\star) + \mathrm{i}k_\star} \sim \frac{1}{(E - E_\star) + \mathrm{i}k_\star \frac{\hbar^2}{ma}}$$

Стандартная запись подобной ам пЛитуды резонанса в виде

$$A \sim \frac{1}{(E - E_\star) + \frac{i}{2}\Gamma}$$

называется приближением Брейта-Вигнера.

Величину Γ называют шириной резонанса.

Квадрат модуля амплитуды -

$$|A|^2 \sim \frac{1}{(\Delta E)^2 + \frac{1}{4}\Gamma^2}$$

так что при $\Delta E = \pm\Gamma/2$ плотность вероятности обнаружения резонанса падает вдвое. Поэтому Γ еще называют шириной на полувысоте. В рассматриваемой нами задаче

$$\Gamma = 2\frac{\hbar^2 k_\star}{ma}$$

Амплитуда Брейта-Вигнера как функция энергии представляет собой полюс в комплексной плоскости энергии при

$$E_{\text{pole}} = E_\star - \frac{\mathrm{i}}{2}\Gamma.$$

Time-dependent scattering on a wall near well (????????)

(???? I'll think later, a big advanced question)

Поэтому считают, что временная зависимость волновой функции резонанса

$$\psi \sim \mathrm{e}^{-\frac{i}{\hbar}E_{\text{pole}}\, t} = \mathrm{e}^{-\frac{i}{\hbar}E_\star t}\mathrm{e}^{-\frac{1}{2\hbar}\Gamma t}$$

имеет затухающий фактор, так что плотность вероятности падает со временем как

$$|\psi|^2 \sim \mathrm{e}^{-\frac{1}{\hbar}\Gamma t}.$$

Величину

$$\tau = \frac{\hbar}{\Gamma}$$

называют временем жизни резонанса. Тогда

$$|\psi|^2 \sim \mathrm{e}^{-t/\tau}.$$

В нашем случае

$$\tau = \frac{ma}{2\hbar k_\star},$$

что находится в полном согласии с приведенной выше интерпретацией времени запаздывания сигнала в терминах комплексной фазы за счет возбуждения резонанса.

2.2. Eigenfunction expansion.

Here we explicitly construct the resolvent kernel for the one-dimensional Schrodinger operator H, and show that it is self-adjoint with the domain consisting of functions $\psi \in L^2(\mathbb{R})$, which are twice differentiable on $\mathbb{R}$, and such that $-\psi'' + V(x)\psi \in L^2(\mathbb{R})$. Using the method of complex integration we derive the eigenfunction expansion theorem for the operator H, which generalizes the corresponding result for the operator H_0 of a free quantum particle, considered in Section 2.3 of Chapter 2.

For $\lambda \in \mathbb{C}\backslash[0,\infty)$ let

$$R_\lambda(x,y) = \begin{cases} -\frac{f_1(x,k)f_2(y,k)}{2ika(k)} & \text{if } x \geq y \\ -\frac{f_1(y,k)f_2(x,k)}{2ika(k)} & \text{if } x \leq y \end{cases} \tag{2.21}$$

where the branch of the function $k = \sqrt{\lambda}$ on $\mathbb{C}\backslash[0,\infty)$ is defined by the condition that $\operatorname{Im} k > 0$. For fixed x and y the function $R_\lambda(x,y)$ is meromorphic on $\mathbb{C}\backslash[0,\infty)$ with simple poles at $\lambda_l = -\varkappa_l^2, l = 1, ..., n$. For fixed
$\lambda \neq \lambda_l$ the function $R_\lambda(x,y) = R_\lambda(y,x)$ is continuous in x and y, and it follows from part (v) of Theorem 2.1 and (2.15) that

$$|R_\lambda(x,y)| \leq C\frac{e^{-\operatorname{Im} k|x-y|}}{|k|}, \quad C > 0. \tag{2.22}$$

The kernel $R_\lambda(x,y)$ for $\lambda \neq \lambda_l$ defines a bounded integral operator R_λ in $L^2(\mathbb{R})$ by the formula

$$\left(R_\lambda\psi\right)(x) = \int_{-\infty}^{\infty} R_\lambda(x,y)\psi(y)dy$$

Indeed, it follows from (2.22) that for $\psi \in L^2(\mathbb{R})$,

$$|k|^2 \left\|R_\lambda\psi\right\|^2 \leq C^2 \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} e^{-\operatorname{Im} k|x-y|}|\psi(y)|dy\right)^2 dx$$
$$= C^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\operatorname{Im} k(|y_1|+|y_2|)} \int_{-\infty}^{\infty} \left|\psi\left(x+y_1\right)\psi\left(x+y_2\right)\right| dxdy_1dy_2$$
$$\leq 4C^2(\operatorname{Im} k)^{-2}\|\psi\|^2$$

In particular,

$$\|R_\lambda\| \le \frac{2C}{|k| \operatorname{Im} k}$$

Lemma 2.1. The operator H is self-adjoint and $R_\lambda = (H - \lambda I)^{-1}$ for $\lambda \in \mathbb{C}\setminus\{[0,\infty) \cup \{\lambda_1, ..., \lambda_n\}\}$, where I is the identity operator in $L^2(\mathbb{R})$.

Proof. Let $g \in L^2(\mathbb{R})$. As in the variation of parameters method, it follows from (2.21) that for $\lambda \in \mathbb{C}\setminus\{[0,\infty) \cup \{\lambda_1, ..., \lambda_n\}\}$ the function $y = R_\lambda g \in L^2(\mathbb{R})$ is twice differentiable a.e. on $\mathbb{R}$ and satisfies the differential equation

$$-y'' + V(x)y = \lambda y + g(x)$$

Thus $(H - \lambda I)R_\lambda = I$ and, in particular, $\operatorname{Im}(H \pm iI) = L^2(\mathbb{R})$, so that H is self-adjoint.

Let $\mathfrak{H}_0$ be the Hilbert space of $\mathbb{C}^2$-valued functions $\Phi(\lambda) = \binom{\varphi_1(\lambda)}{\varphi_2(\lambda)}$ on $[0,\infty)$ with the norm

$$\|\Phi\|_0^2 = \int_0^\infty \left(|\varphi_1(\lambda)|^2 + |\varphi_2(\lambda)|^2\right) d\sigma(\lambda)$$

where $d\sigma(\lambda) = \frac{1}{2\sqrt{\lambda}} d\lambda$ and $\sqrt{\lambda} \ge 0$ for $\lambda \ge 0$ (see Section 2.3 of Chapter 2, where one should put $\hbar = 1$ and $m = \frac{1}{2}$). For $\lambda \ge 0$ set

$$u_j(x, \sqrt{\lambda}) = \frac{1}{a(\sqrt{\lambda})} f_j(x, \sqrt{\lambda}), \quad j = 1, 2 \tag{2.23}$$

and for $\psi \in C_0^2(\mathbb{R})$ define the $\mathbb{C}^2$-valued function $\mathscr{U}\psi$ on $[0,\infty)$ with components $(\mathscr{U}\psi)_1$ and $(\mathscr{U}\psi)_2$ by

$$(\mathscr{U}\psi)_j(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty \psi(x)\overline{u_j(x, \sqrt{\lambda})} dx, \quad j = 1, 2. \tag{2.24}$$

By Proposition 2.1 the function $\mathscr{U}\psi$ is bounded at $\lambda = 0$, and for large λ using differential equation (2.1) and integration by parts we get

$$(\mathscr{U}\psi)_j(\lambda) = \frac{1}{\lambda\sqrt{2\pi}} \int_{-\infty}^\infty (-\psi''(x) + V(x)\psi(x))\, \overline{u_j(x, \sqrt{\lambda})} dx$$

which shows that $\mathscr{U}\psi \in \mathfrak{H}_0$.

Let P be the orthogonal projection on the subspace of $\mathscr{H} = L^2(\mathbb{R})$ spanned by the eigenfunctions $\psi_l(x) = f_1(x, i\varkappa_l), l = 1, ..., n$. The functions ψ_l are real-valued and orthogonal, so that for $\psi \in \mathscr{H}$

$$(P\psi)(x) = \sum_{l=1}^n \frac{1}{\|\psi_l\|^2} \psi_l(x) \int_{-\infty}^\infty \psi(y)\psi_l(y) dy$$

Theorem 2.3. The operator $\mathscr{U}$ extends to a partial isometry operator $\mathscr{U}\colon \mathscr{H} \to \mathfrak{H}_0$,

$$\mathscr{U}^*\mathscr{U} = I - P \quad \text{and} \quad \mathscr{U}\mathscr{U}^* = I_0,$$

and establishes the isomorphism $(I - P)\mathscr{H} \simeq \mathfrak{H}_0$. Here I and I_0 are, respectively, identity operators in $\mathscr{H}$ and $\mathfrak{H}_0$. For the spectrum of the corresponding Schrodinger operator H we have $\sigma(H) = \{-\varkappa_1^2, ..., -\varkappa_n^2\} \cup [0,\infty)$, and

$$\mathscr{H} = \mathscr{H}_{\text{pp}} \oplus \mathscr{H}_{\text{ac}}$$

where $\mathscr{H}_{\text{pp}} = P\mathscr{H}$ and $\mathscr{H}_{\text{ac}} = (I - P)\mathscr{H}$ are, respectively, invariant subspaces associated with pure point and absolutely continuous spectra of H. The operator $\mathscr{U} H_{\mathscr{U}^*}$ is a multiplication

by λ operator in $\mathfrak{H}_0$, so that the absolutely continuous spectrum $[0,\infty)$ of H has multiplicity two, and the operator $\mathscr{U}$ "diagonalizes" the restriction of H to the subspace $\mathscr{H}_{\rm ac}$.

Proof. To proof the relation $\mathscr{U}^*\mathscr{U} = I - P^-$ the so-called completeness relation - it is sufficient to establish the following classical eigenfunction expansion formula for $\psi \in C_0^2(\mathbb{R})$:
$\psi(x) = \frac{1}{2\pi}\int_0^\infty \left(u_1(x,k)\int_{-\infty}^\infty \psi(y)\overline{u_1(y,k)}dy + u_2(x,k)\int_{-\infty}^\infty \psi(y)\overline{u_2(y,k)}dy\right)dk$

$$+\sum_{l=1}^n \frac{1}{\|\psi_l\|^2}\psi_l(x)\int_{-\infty}^\infty \psi(y)\psi_l(y)dy \tag{2.25}$$

where all integrals are absolutely convergent, and we put $\sqrt{\lambda} = k, d\sigma(\lambda) = dk$. Indeed, assuming that (2.25) holds, we get for $\psi, \varphi \in C_0^2(\mathbb{R})$

$$\begin{aligned}(\psi,\varphi) &= \int_{-\infty}^\infty \psi(x)\overline{\varphi(x)}dx = \frac{1}{2\pi}\int_{-\infty}^\infty \overline{\varphi(x)}\left(\int_0^\infty \left(u_1(x,k)\int_{-\infty}^\infty \psi(y)\overline{u_1(y,k)}dy\right.\right.\\ &\left.\left.+u_2(x,k)\int_{-\infty}^\infty \psi(y)\overline{u_2(y,k)}dy\right)dk\right)dx + \sum_{l=1}^n \frac{1}{\|\psi_l\|^2}(\psi,\psi_l)(\psi_l,\varphi)\\ &= (\mathscr{U}\psi,\mathscr{U}\varphi)_0 + \sum_{l=1}^n \frac{1}{\|\psi_l\|^2}(\psi,\psi_l)(\psi_l,\varphi)\end{aligned}$$

where $(,)_0$ is the inner product in $\mathfrak{H}_0$, and the interchange of integrals over x and k is justified by the Fubini theorem. Thus

$$(\mathscr{U}\psi,\mathscr{U}\varphi)_0 = ((I-P)\psi,\varphi) \tag{2.26}$$

for $\psi, \varphi \in C_0^2(\mathbb{R})$, and we conclude that $\mathscr{U}$ extends to a bounded operator from $\mathscr{H}$ and $\mathfrak{H}_0$ satisfying (2.26) for all $\psi, \varphi \in \mathscr{H}$.

To prove the eigenfunction expansion formula (2.25), for $\lambda \in \mathbb{C}\backslash[0,\infty)$ set $g(x,\lambda) = (R_\lambda\psi)(x)$. The function $g(x,\lambda)$ for fixed x is meromorphic in $\lambda \in \mathbb{C}\backslash[0,\infty)$ with simple poles at $\lambda = \lambda_l, l = 1,...,n$. It follows from (2.21) and Proposition 2.1 that

$$\mathrm{Res}_{\lambda=\lambda_l} g(x,\lambda) = \frac{ic_l}{\dot{a}(i\varkappa_l)}f_2(x,i\varkappa_l)\int_{-\infty}^\infty f_2(y,i\varkappa_l)\psi(y)dy = -\frac{(\psi,\psi_l)}{\|\psi_l\|^2}\psi_l(x)$$

Since $HR_\lambda = R_\lambda H = I + \lambda R_\lambda$, we have

$$-g''(x,\lambda) + V(x)g(x,\lambda) = \psi(x) + \lambda g(x,\lambda)$$

so that

$$g(x,\lambda) = -\frac{1}{\lambda}\psi(x) + \frac{1}{\lambda}(R_\lambda\varphi)(x)$$

where $\varphi = -\psi'' + V(x)\psi \in C_0(\mathbb{R})$. From (2.22) we get

$$|(R_\lambda\varphi)(x)| \le \frac{C}{|\sqrt{\lambda}|} \quad \text{as} \quad |\lambda| \to \infty$$

so that

$$g(x,\lambda) = -\frac{1}{\lambda}\psi(x) + O\left(|\lambda|^{-3/2}\right) \quad \text{as} \quad |\lambda| \to \infty \tag{2.27}$$

It follows from Proposition 2.1 and (2.21) that

$$g(x,\lambda) = O\left(|\lambda|^{-1/2}\right) \quad \text{as} \quad \lambda \to 0 \tag{2.28}$$

For $0 < \varepsilon < 1 < N$ let $\mathcal{C} = \mathcal{C}_{\varepsilon,N}$ be the contour consisting of the following parts: (i) the arc $\mathcal{C}_\varepsilon$ of a circle $\lambda = \varepsilon e^{i\theta}, \varepsilon \le |\arg\theta| \le \pi$, oriented clockwise; (ii) the arc $\mathcal{C}_N$ of a circle $\lambda = Ne^{i\theta}, \varepsilon_N \le |\arg\theta| \le \pi$, oriented anti-clockwise, where $N\sin\varepsilon_N = \varepsilon\sin\varepsilon$; (iii) the segments $\mathcal{I}_\pm$of the straight
lines $\operatorname{Im}\lambda = \pm\varepsilon\sin\varepsilon$ which connect the boundaries of the arcs. Choose ε and N such that all poles λ_l of $g(x,\lambda)$ are inside $\mathcal{C}$, and consider the integral

$$I = \frac{1}{2\pi i}\int_{\mathcal{C}} g(x,\lambda)d\lambda$$

On one hand, by the Cauchy residue theorem

$$I = \sum_{l=1}^{n} \operatorname{Res}_{\lambda=\lambda_l} g(x,\lambda) = -\sum_{l=1}^{n} \frac{(\psi,\psi_l)}{\|\psi_l\|^2}\psi_l(x)$$

On the other hand, it follows from (2.27) and (2.28) that

$$\lim_{N\to\infty}\frac{1}{2\pi i}\int_{\mathcal{C}_N} g(x,\lambda)d\lambda = -\psi(x) \quad \text{and} \quad \lim_{\varepsilon\to 0}\frac{1}{2\pi i}\int_{\mathcal{C}_\varepsilon} g(x,\lambda)d\lambda = 0$$

Thus we obtain

$$\begin{aligned}\psi(x) - \sum_{l=1}^{n}\frac{1}{\|\psi_l\|^2}(\psi,\psi_l)\psi_l(x) &= \lim_{\varepsilon\to 0}\lim_{N\to\infty}\frac{1}{2\pi i}\left(\int_{\mathcal{I}_+} g(x,\lambda)d\lambda - \int_{\mathcal{I}_-} g(x,\lambda)d\lambda\right)\\ &= \frac{1}{2\pi i}\int_0^\infty\left(\int_{-\infty}^{\infty}\left(R_{\lambda+i0}(x,y) - R_{\lambda-i0}(x,y)\right)\psi(y)dy\right)d\lambda, \qquad (2.29)\end{aligned}$$

where

$$R_{\lambda\pm i0}(x,y) = \lim_{\varepsilon\to 0} R_{\lambda\pm i\varepsilon}(x,y)$$

To compute the difference $R_{\lambda+i0}(x,y) - R_{\lambda-i0}(x,y)$, observe that on the cut $\lambda \ge 0$ we have $\sqrt{\lambda+i0} = k \ge 0$ and $\sqrt{\lambda-i0} = -k \le 0$. It follows from (2.21) that for $x \ge y$
$R_{\lambda+i0}(x,y) - R_{\lambda-i0}(x,y) = -\frac{1}{2ik}\left(\frac{f_1(x,k)f_2(y,k)}{a(k)} + \frac{f_1(x,-k)f_2(y,-k)}{a(-k)}\right)$,
and using the equations

$$\begin{aligned}f_1(x,k) &= \frac{1}{a(-k)}f_2(x,-k) - \frac{b(-k)}{a(-k)}f_1(x,-k),\\ f_2(y,-k) &= \frac{1}{a(k)}f_1(y,k) + \frac{b(-k)}{a(k)}f_2(y,k),\end{aligned}$$

which follow from (2.11) and (2.13), we obtain

$$\begin{aligned}R_{\lambda+i0}(x,y) - R_{\lambda-i0}(x,y) &= \frac{i}{2k|a(k)|^2}\left(f_1(x,k)\overline{f_1(y,k)} + f_2(x,k)\overline{f_2(y,k)}\right)\\ &= \frac{i}{2k}\left(u_1(x,k)\overline{u_1(y,k)} + u_2(x,k)\overline{u_2(y,k)}\right)\end{aligned}$$

where $\lambda = k^2$. Substituting this into (2.29) and using the symmetry $R_\lambda(x,y) = R_\lambda(y,x)$ of the resolvent kernel, we get the eigenfunction expansion (2.25).

Let $\mathscr{U}_{\rm ac}$ be the restriction of the operator $\mathscr{U}$ to the subspace $\mathscr{H}_{\rm ac} = (I-P)\mathscr{H}$. It follows from the completeness relation that the operator $\mathscr{U}_{\rm ac}$

is an isometry, so that $\mathrm{Im}\,\mathscr{U} = \mathrm{Im}\,\mathscr{U}_{\mathrm{ac}}$ is a closed subspace of $\mathfrak{H}_0$. Thus to verify the orthogonality relation $\mathscr{U}\mathscr{U}^* = I_0$, it is sufficient to show that $\mathrm{Im}\,\mathscr{U} = \mathfrak{H}_0$. Using integration by parts we easily get that a self-adjoint operator $\mathscr{U}_{\mathrm{ac}} H \mathscr{U}_{\mathrm{ac}}^{-1}$ is a multiplication by λ operator in $\mathrm{Im}\,\mathscr{U}$ with the domain $\mathscr{U}D(H)$. Moreover,

$$\mathscr{U}R_\mu = R_\mu^{(0)}\mathscr{U}, \quad \mu \in \mathbb{C}\backslash[0,\infty),$$

where $R_\mu^{(0)}$ is the resolvent of the multiplication by λ operator in $\mathfrak{H}_0$, so that $\mathrm{Im}\,\mathscr{U}$ is an invariant subspace for $R_\mu^{(0)}$. Now it follows from Lemma 2.2 in Section 2.2 of Chapter 2 that there are Borel subsets $E_1, E_2 \subseteq [0,\infty)$ such that

$$\mathrm{Im}\,\mathscr{U} = \left\{ \tilde{\Phi} = \begin{pmatrix} \chi_{E_1}\varphi_1 \\ \chi_{E_2}\varphi_2 \end{pmatrix}, \quad \Phi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \in \mathfrak{H}_0 \right\}.$$

If, say, $E_1^{\mathrm{c}} = [0,\infty)\backslash E_1$ has positive Lebesgue measure, then for $\lambda = k^2 \in E_1^{\mathrm{c}}$ we have

$$\int_{-\infty}^{\infty} \overline{u_1(x,k)}\psi(x)dx = 0 \quad \text{for all} \quad \psi \in C_0^2(\mathbb{R}),$$

so that $u(x,k) = 0$ for all $x \in \mathbb{R}$ - a contradiction. Therefore, $\mathrm{Im}\,\mathscr{U} = \mathfrak{H}_0$.

Let $\mathscr{U}_0 : \mathscr{H} \to \mathfrak{H}_0$ be the corresponding unitary operator for the Schrodinger operator H_0 of a free particle, constructed in Section 2.3 of Chapter 2 (with $\hbar = 1$ and $m = \frac{1}{2}$), and set $U = \mathscr{U}^*\mathscr{U}_0 : \mathscr{H} \to \mathscr{H}_{\mathrm{ac}}$.

Corollary 2.4. The restriction of H to the absolutely continuous subspace $\mathscr{H}_{\mathrm{ac}}$ is unitarily equivalent to H_0,

$$H|_{\mathscr{H}_{\mathrm{ac}}} = UH_0U^{-1}.$$

Remark. In physics literature, completeness and orthogonality relations, understood in the distributional sense, are usually written as

$$\frac{1}{2\pi}\int_0^\infty \left(u_1(x,k)\overline{u_1(y,k)} + u_2(x,k)\overline{u_2(y,k)} \right) dk + \sum_{l=1}^{n} \frac{\psi_l(x)\psi_l(y)}{\|\psi_l\|^2} = \delta(x-y)$$

and

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} u_j(x,k)\overline{u_k(x,p)}dx = \delta_{jk}\delta(k-p),$$

where $i,k = 1,2$ and $k,p > 0$. When transition coefficients $a(k)$ and $b(k)$ are differentiable for $k \neq 0$[2], the orthogonality relation can be derived from the identity

$$\frac{d}{dx}W\left(u_j(x,k), \overline{u_k(x,p)}\right) = \left(k^2 - p^2\right) u_j(x,k)\overline{u_k(x,p)}, \tag{2.30}$$

which immediately follows from the differential equation (2.1). Namely, consider the case $j = k = 1$ and integrate (2.30) over $[-N,N]$. Using (2.13) and asymptotics of Jost solutions, we get

[2] This is the case when $V(x)$ satisfies $\int_{-\infty}^{\infty}\left(1+|x|^2\right)|V(x)|dx < \infty$.

$$\int_{-N}^{N} u_1(x,k)\overline{u_1(x,p)}dx = \frac{1}{(k^2-p^2)\,a(k)\overline{a(p)}} W\left(f_1(x,k), \overline{f_1(x,p)}\right)\Big|_{-N}^{N}$$
$$= \frac{i}{a(k)\overline{a(p)}}\left(\frac{e^{i(k-p)N} - a(k)\overline{a(p)}e^{-i(k-p)N} + \overline{b(k)}b(p)e^{i(k-p)N}}{k-p}\right.$$
$$\left. + \frac{a(k)b(p)e^{-i(k+p)N} - \overline{b(k)a(p)}e^{i(k+p)N}}{k+p}\right) + o(1) \quad \text{as} \quad N\to\infty$$

Since $k, p > 0$, by the Riemann-Lebesgue lemma the distributional limit as $N \to \infty$ of the terms in the third line is zero. Since $a(k)$ and $b(k)$ are assumed differentiable, in the second line we can replace $\overline{a(p)}$ and $b(p)$ by $\overline{a(k)}$ and $b(k)$, respectively, since the difference goes to zero as $N \to \infty$ by the Riemann-Lebesgue lemma. Finally, using (2.14) we obtain

$$\lim_{N\to\infty}\int_{-N}^{N} u_1(x,k)\overline{u_1(x,p)}dx = 2\lim_{N\to\infty}\frac{\sin(k-p)N}{k-p} = 2\pi\delta(k-p),$$

where the last equality is the distributional form of the orthogonality relation for the Fourier transform.

Remark. The eigenfunctions of the continuous spectrum $u_j(x,\lambda)$ also satisfy the normalization condition (2.14) in Section 2.2 of Chapter 2:

$$\lim_{\Delta\to 0}\frac{1}{\Delta}\left(U_{j,k+\Delta} - U_{j,k}, U_{l,k+\Delta} - U_{l,k}\right) = \delta_{jl}, \quad j,l = 1,2$$

where

$$U_{j,k}(x) = \int_{k_0^2}^{k^2} u_j(x,\sqrt{\lambda})\frac{d\lambda}{2\sqrt{\lambda}} = \int_{k_0}^{k}\frac{f_j(x,p)}{a(p)}dp, \quad j = 1,2.$$

Remark. The qualitative structure of the spectrum of the Schrodinger operator H is determined by the structure of the level sets $H_c(p,x) = \lambda$ of the classical Hamiltonian function $H_c(p,x) = p^2 + V(x)$. Namely, condition $\lim_{|x|\to\infty} V(x) = 0$ implies that the level sets for $\lambda > 0$ are non-compact and the classical motion is unbounded in both directions, and these values of λ fill the absolutely continuous spectrum $[0,\infty)$ of H of multiplicity two. For $\lambda < 0$ the level sets are compact and classical motion is periodic. According to BWS quantization rules (see Section 2.5 in Chapter 2), the energy levels - eigenvalues of H - correspond to the closed orbits, and condition (2.2) guarantees that H has only finitely many eigenvalues.

Problem 2.5. Find the energy levels for the potential

$$V(x) = -\frac{V_0}{\cosh^2 \varkappa x}, \quad V_0 > 0.$$

In particular, show that when $V_0 = 2\varkappa^2$ there is only one eigenvalue $E = -\varkappa^2$.

Problem 2.6. Show that the operator $R_\lambda - R_\lambda^{(0)}$, where $R_\lambda^{(0)} = (H_0 - \lambda I)^{-1}$ and $\lambda \in \mathbb{C}\backslash[0,\infty)$, is of the trace class, and

$$\mathrm{Tr}\left(R_\lambda - R_\lambda^{(0)}\right) = -\frac{d}{d\lambda}\log a(\sqrt{\lambda}).$$

(Hint: Use Wronskian identities (2.19)-(2.20) from the previous section.)

2.3. S-matrix and scattering theory.

It was shown in the previous section that for potentials $V(x)$ satisfying (2.2) the operators $H = H_0 + V$ and H_0 have the same absolutely continuous spectrum. Among many partial isometry operators in $\mathscr{H}$ which establish the unitary equivalence between $H|_{\mathscr{H}_{\rm ac}}$ and H_0, there are two operators $W_\pm$of fundamental physical significance. They are defined as

$$W_\pm = \lim_{t\to\pm\infty} e^{iHt}e^{-itH_0} \tag{2.31}$$

where the limit is understood in the strong operator topology, and are called wave operators (or Mller operators). In general, the wave operators exist for a Schrodinger operator $H = H_0+V$ on $\mathbb{R}^n$ with the potential $V(\boldsymbol{q})$ decaying sufficiently fast as $|\boldsymbol{q}| \to \infty$. In this section, we will show that for potentials $V(x)$ satisfying (2.2) the limits (2.31) exist.

The wave operators satisfy the partial isometry relation

$$W_\pm^* W_\pm = I \tag{2.32}$$

Indeed, strong limits of unitary operators preserve the inner products, so that $(W_\pm\psi, W_\pm\varphi) = (\psi,\varphi)$ for all $\psi,\varphi \in \mathscr{H}$. Convergence $A_n \to A$ as $n \to \infty$ in the strong operator topology does not necessarily imply that $A_n^* \to A^*$, so that we cannot conclude that $W_\pm W_\pm^* = I$. Thus in general the wave operators are not unitary. In fact, it can be shown that $\operatorname{Im} W_\pm = \mathscr{H}_{\rm ac} = (I-P)\mathscr{H}$ or, equivalently,

$$W_\pm W_\pm^* = I - P \tag{2.33}$$

where P is the orthogonal projection on the subspace $\mathscr{H}_{\rm pp}$. Though the proof of (2.33) is rather non-trivial, it is easy to show that $\operatorname{Im} W_\pm \subseteq (I-P)\mathscr{H}$. Indeed, let $\psi \in \mathscr{H}$ be a bound state - an eigenvector for H,

$$H\psi = \lambda\psi$$

Then for every $\varphi \in \mathscr{H}$ we have

$$(W_\pm\varphi,\psi) = \lim_{t\to\pm\infty} e^{i\lambda t}\left(e^{-itH_0}\varphi,\psi\right) = 0$$

by the Riemann-Lebesgue lemma, as we have seen in Section 2.3 of Chapter 2.

Assuming that wave operators exist and satisfy (2.33), it is easy to prove that

$$f(H)W_\pm = W_\pm f(H_0) \tag{2.34}$$

for any measurable function f on $\mathbb{R}$. Indeed, according to the spectral theorem, it is sufficient to prove this property for the functions $f(\lambda) = e^{i\tau\lambda}$ for all $\tau \in \mathbb{R}$. In this case, (2.34) immediately follows from the identity

$$e^{i\tau H}e^{i(t-\tau)H}e^{-i(t-\tau)H_0} = e^{itH}e^{-itH_0}e^{i\tau H_0}$$

by passing to the limits $t \to \pm\infty$. Using (2.34) and (2.32) we conclude

$$W_\pm^* H W_\pm = H_0$$

so that restrictions of the wave operators to the subspace $\mathscr{H}_{\rm ac}$ establish the unitary equivalence between $H|_{\mathscr{H}_{\rm ac}}$ and H_0.

Remark. The physical meaning of the wave operators is the following. The one-parameter group $U(t) = e^{-itH}$ of unitary operators describes the evolution of the quantum particle moving in a short-ranged potential field. For large $|t|$ the particle with positive energy moves far

away from the center and as $|t| \to \infty$ its evolution is described by the one-parameter group $U_0(t) = e^{-itH_0}$ which corresponds to the free motion. Mathematically this is expressed by the fact that for every $\varphi_- \in \mathscr{H}$ there exists a vector $\psi \in \mathscr{H}$ such that

$$\lim_{t\to-\infty} \left\| e^{-itH}\psi - e^{-itH_0}\varphi_- \right\| = 0$$

and such a vector is given by $\psi = W_-\varphi_-$. Similarly, for every $\varphi_+ \in \mathscr{H}$ the vector $\psi = W_+\varphi_+$satisfies

$$\lim_{t\to\infty} \left\| e^{-itH}\psi - e^{-itH_0}\varphi_+ \right\| = 0$$

As a physical interpretation, orthogonality of $\operatorname{Im} W_\pm$to the subspace $\mathscr{H}_{\rm pp}$ is explained by the fact that for all times t bound states are localized near the potential center, whereas the free quantum particle goes to infinity as $|t| \to \infty$.

The wave operators are used to describe the scattering of the quantum particle by the potential center. Namely, given $\varphi_- \in \mathscr{H}$, there is $\psi = W_-\varphi_- \in \mathscr{H}$ such that the solution $\psi(t) = U(t)\psi$ of the non-stationary Schrodinger equation with Hamiltonian H and initial condition $\psi(0) = \psi$ as $t \to -\infty$ approaches the solution $\varphi_-(t) = U_0(t)\varphi_-$of the non-stationary Schrodinger equation with free Hamiltonian H_0 and initial condition $\varphi_-(0) = \varphi_-$. Since $\operatorname{Im} W_- = \operatorname{Im} W_+$, there is $\varphi_+ \in \mathscr{H}$ such that $\psi = W_+\varphi_+$and
the solution $\psi(t)$ of the non-stationary Schrodinger equation with Hamiltonian H and initial condition $\psi(0) = \psi$ as $t \to \infty$ approaches the solution $\varphi_+(t) = U_0(t)\varphi_+$of the non-stationary Schrodinger equation with free Hamiltonian H_0 and initial condition $\varphi_+(0) = \varphi_+$. The passage from the solution $\varphi_-(t)$ of the free Schrodinger equation describing the motion of quantum particle at $t = -\infty$ to the solution $\varphi_+(t)$ describing its motion at $t = \infty$ is the result of scattering of the quantum particle by a potential center. All information about the scattering is contained in the scattering operator S (also called S-matrix in physics), which relates initial and final conditions $\varphi_-$and φ_+:

$$\varphi_+ = S\varphi_-$$

From (2.32) and $\psi = W_-\varphi_- = W_+\varphi_+$we immediately get that

$$S = W_+^* W_-, \tag{2.35}$$

and from (2.32)-(2.34) we obtain that the scattering operator S is a unitary operator in $\mathscr{H}$ and commutes with the free Hamiltonian H_0:

$$S^*S = SS^* = I \quad \text{and} \quad SH_0 = H_0S$$

This is the outline of a non-stationary approach to scattering theory.
In the stationary approach to scattering theory, the wave operators $W_\pm$ and the scattering operator S are constructed as integral operators in the coordinate representation with integral kernels expressed through special solutions of the stationary Schrodinger equation. Here we present this construction for the one-dimensional Schrodinger operator considered in the previous section.

Namely, let $u_1(x,k)$ and $u_2(x,k)$ be solutions of the one-dimensional Schrodinger equation (2.1) given by (2.23), where $\sqrt{\lambda} = k > 0$. It follows from Theorem 2.1 and (2.11), (2.13) that these solutions have the following asymptotics:

$$\begin{aligned} u_1(x,k) &= s_{11}(k)e^{ikx} + o(1) && \text{as} \quad x \to \infty \\ u_1(x,k) &= e^{ikx} + s_{21}(k)e^{-ikx} + o(1) && \text{as} \quad x \to -\infty \end{aligned} \tag{2.37}$$

and

$$\begin{array}{lll} u_2(x,k) = e^{-ikx} + s_{12}(k)e^{ikx} + o(1) & \text{as} & x \to \infty \\ u_2(x,k) = s_{22}(k)e^{-ikx} + o(1) & \text{as} & x \to -\infty \end{array} \tag{2.39}$$

where

$$s_{11}(k) = s_{22}(k) = \frac{1}{a(k)}, \quad s_{12}(k) = \frac{b(k)}{a(k)}, \quad s_{21}(k) = -\frac{\overline{b(k)}}{a(k)}. \tag{2.40}$$

Solutions $u_1(x,k)$ and $u_2(x,k)$ are called scattering solutions, the function $s_{11}(k)$ is called the complex transmission coefficient, and functions $s_{12}(k)$ and
$s_{21}(k)$, respectively, are called right and left complex reflection coefficients. Correspondingly, $T = |s_{11}(k)|^2$ is called the transmission coefficient and $R = |s_{12}(k)|^2 = |s_{21}(k)|^2$ - the reflection coefficient. The 2×2 matrix

$$S(k) = \begin{pmatrix} s_{11}(k) & s_{12}(k) \\ s_{21}(k) & s_{22}(k) \end{pmatrix}$$

is called the scattering matrix. It follows from (2.14) that the scattering matrix is unitary, $S^*(k)S(k) = I$, where I is the 2×2 identity matrix, and satisfies $\overline{S(k)} = S(-k)$. In particular, unitarity of the scattering matrix implies that $T + R = 1$, which is called conservation of probability.

The physical interpretation of the solutions $u_1(x,k)$ and $u_2(x,k)$ is the following. For simplicity, suppose that the potential $V(x)$ is smooth and vanishes for $|x| > A$, so that asymptotics (2.36) and (2.38) become equalities for $x > A$, and asymptotics (2.37) and (2.39) become equalities for $x < -A$. In this case elements $s_{ij}(k)$ of the scattering matrix are smooth functions for $k \neq 0$. As in Section 2.3 of Chapter 2, let $\varphi_1(k)$ and $\varphi_2(k)$ be the wave packets: smooth functions on $(0, \infty)$ supported in some neighborhood U_0 of $k_0 > 0$. The functions, called scattering waves,

$$\psi_j(x,t) = \int_0^\infty \varphi_j(k)u_j(x,k)e^{-ik^2t}dk, \quad j = 1,2$$

are solutions of the time-dependent Schrodinger equation

$$i\frac{\partial \psi}{\partial t} = H\psi$$

In the region $|x| > A$ the solution $\psi_1(x,t)$ can be simplified as follows:

$$\begin{array}{ll} \psi_1(x,t) = \int_0^\infty \varphi_1(k)s_{11}(k)e^{ikx-ik^2t}dk, & \text{when} \quad x > A \\ \psi_1(x,t) = \int_0^\infty \varphi_1(k)\left(e^{ikx-ik^2t} + s_{21}(k)e^{-ikx-ik^2t}\right)dk, & \text{when} \quad x < -A \end{array}$$

Using the method of stationary phase (see Section 2.3 in Chapter 2) we get as $t \to -\infty$,

$$\begin{array}{ll} \psi_1(x,t) = O\left(|t|^{-1}\right), & \text{when } x > A \\ \psi_1(x,t) = \frac{1}{\sqrt{|t|}}\varphi_1\left(\frac{x}{2t}\right)e^{\frac{ix}{2}x^2 + \frac{i\pi}{4}} + O\left(|t|^{-1}\right), & \text{when } x < -A \end{array}$$

and as $t \to \infty$,

$$\begin{array}{ll} \psi_1(x,t) = \frac{1}{\sqrt{t}}\varphi_1\left(\frac{x}{2t}\right)s_{11}\left(\frac{x}{2t}\right)e^{\frac{ix^2}{4t} - \frac{i\pi}{4}} + O\left(t^{-1}\right), & \text{when} \quad x > A \\ \psi_1(x,t) = \frac{1}{\sqrt{t}}\varphi_1\left(-\frac{x}{2t}\right)s_{21}\left(-\frac{x}{2t}\right)e^{\frac{ix^2}{4t} - \frac{i\pi}{4}} + O\left(t^{-1}\right), & \text{when} \quad x < -A \end{array}$$

Assuming that the neighborhood U_0 is "sufficiently small", we see as in Section 2.3 of Chapter 2 that as $t \to -\infty$ the solution $\psi_1(x,t)$ represents a plane wave with amplitude

$|\varphi_1(k_0)|$ moving from $x=-\infty$ to the right, toward the potential center, with velocity $v=2k_0$. When $t\to\infty$, the solution $\psi_1(x,t)$ is a superposition of two plane waves: the transmitted wave with amplitude $|s_{11}(k_0)|$ times the original amplitude, located to the right of the potential center and moving toward ∞ with velocity v, and the reflected wave with amplitude factor $|s_{21}(k_0)|$, located to the left of the potential center and moving toward $-\infty$ with velocity $-v$. Corresponding transmission and reflection coefficients are $T=|s_{11}(k_0)|^2$ and $R=|s_{21}(k_0)|^2$.

Analogously, we have as $t\to-\infty$,

$$\begin{aligned}\psi_2(x,t)&=\tfrac{1}{\sqrt{|t|}}\varphi_2\left(-\tfrac{x}{2t}\right)e^{\frac{ix^2}{4t}-\frac{i\pi}{4}}+O\left(|t|^{-1}\right), &&\text{when}\quad x>A\\ \psi_2(x,t)&=O\left(|t|^{-1}\right), &&\text{when}\quad x<-A\end{aligned}$$

and as $t\to\infty$,

$$\begin{aligned}\psi_2(x,t)&=\frac{1}{\sqrt{t}}\varphi_2\left(\frac{x}{2t}\right)s_{12}\left(\frac{x}{2t}\right)e^{\frac{ix^2}{4t}-\frac{i\pi}{4}}+O\left(t^{-1}\right), &&\text{when}\quad x>A\\ \psi_2(x,t)&=\frac{1}{\sqrt{t}}\varphi_2\left(-\frac{x}{2t}\right)s_{22}\left(-\frac{x}{2t}\right)e^{\frac{ix^2}{4t}-\frac{i\pi}{4}}+O\left(t^{-1}\right), &&\text{when}\quad x<-A.\end{aligned}$$

As $t\to-\infty$, the solution $\psi_2(x,t)$ is a plane wave with amplitude $|\varphi_2(k_0)|$ moving from $x=\infty$ to the left, toward the potential center, with velocity $-v$. When $t\to\infty$, the solution $\psi_2(x,t)$ is a superposition of two plane waves: the transmitted wave with the same amplitude factor $|s_{22}(k_0)|$, located to the left of the potential center and moving toward $-\infty$ with velocity $-v$, and the reflected wave with amplitude factor $|s_{12}(k_0)|$, located to the right of the potential center and moving toward ∞ with velocity v. Formulas (2.40) show that transmission and reflection coefficients for the solution $\psi_2(x,t)$ are the same as for the solution $\psi_1(x,t)$, and are independent of the direction of travel. This is the so-called reciprocity property of the transmission coefficient.

The solutions $u_1(x,k)$ and $u_2(x,k)$ of the stationary Schrodinger equation have the property that corresponding solutions $\psi_1(x,t)$ and $\psi_2(x,t)$ of the time-dependent Schrodinger equation become the plane waves as $t\to-\infty$. In accordance with this interpretation, we denote them, respectively, by $u_1^{(-)}(x,k)$ and $u_2^{(-)}(x,k)$. Solutions of the stationary Schrodinger equation, $u_1^{(+)}(x,k)=\overline{u_2(x,k)}=u_2(x,-k)$ and $u_2^{(+)}(x,k)=\overline{u_1(x,k)}=u_1(x,-k)$, admit a similar interpretation: they correspond to the solutions of the timedependent Schrodinger equation which become the plane waves as $t\to\infty$.

Introducing

$$U_+(x,k)=\begin{pmatrix}u_1^{(+)}(x,k)\\ u_2^{(+)}(x,k)\end{pmatrix}\quad\text{and}\quad U_-(x,k)=\begin{pmatrix}u_1^{(-)}(x,k)\\ u_2^{(-)}(x,k)\end{pmatrix}$$

we get by a straightforward computation using (2.11) and (2.13) that

$$U_+(x,k)=\overline{S(k)}U_-(x,k) \tag{2.41}$$

The following result establishes equivalence between stationary and nonstationary approaches to scattering theory.

Theorem 2.5. For the one-dimensional Schrodinger operator $H=H_0+V$ with potential $V(x)$ satisfying condition (2.2) the wave operators exist and are given explicitly by

$$W_\pm=\mathscr{U}_\pm^*\mathscr{U}_0$$

Here $\mathscr{U}_\pm:\mathscr{H}\to\mathfrak{H}_0$ are the integral operators given by

$$\mathscr{U}_\pm(\psi)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(x)\overline{U_\pm(x,\sqrt{\lambda})}dx$$

and $\mathscr{U}_0 : \mathscr{H} \to \mathfrak{H}_0$ establishes the unitary equivalence between the operator H_0 in $\mathscr{H}$ and the multiplication by λ operator in $\mathfrak{H}_0$,

$$\mathscr{U}_0(\psi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) \begin{pmatrix} e^{-i\sqrt{\lambda}x} \\ e^{i\sqrt{\lambda}x} \end{pmatrix} dx$$

The scattering operator S in $\mathscr{H}$ and the multiplication by the scattering matrix $S(\sqrt{\lambda})$ operator in $\mathfrak{H}_0$ are unitarily equivalent:

$$S = \mathscr{U}_0^* S(\sqrt{\lambda}) \mathscr{U}_0$$

Proof. The formula for the scattering operator immediately follows from the definition of the operators $\mathscr{U}_\pm$, formula (2.41), and orthogonality relation $\mathscr{U}_- \mathscr{U}_-^* = I_0$ (see Theorem 2.3). To prove that $W_\pm = \mathscr{U}_\pm^* \mathscr{U}_0$, it is sufficient to show that for all $\Phi = \binom{\varphi_1}{\varphi_2} \in \mathfrak{H}_0$, where $\varphi_1(k)$ and $\varphi_2(k)$ are smooth functions on $(0, \infty)$ with compact support,

Indeed, setting $\chi^{(\pm)}(t) = \left(e^{-itH} \mathscr{U}_\pm^* - e^{-itH_0} \mathscr{U}_0^*\right) \Phi$, we have

$$\chi^{(\pm)}(x,t) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \left(\left(u_1^{(\pm)}(x,k) - e^{ikx} \right) \varphi_1(k) + \left(u_2^{(\pm)}(x,k) - e^{-ikx} \right) \varphi_2(k) \right) e^{-ik^2 t} dk$$

and it is not difficult to estimate the integral

$$\left\| \chi^{(\pm)}(t) \right\|^2 = \int_{-\infty}^{\infty} \left| \chi^{(\pm)}(x,t) \right|^2 dx \tag{2.42}$$

as $t \to \pm\infty$. Namely, it follows from the Riemann-Lebesgue lemma that for any fixed $A > 0$ the contribution to (2.42) from the interval $[-A, A]$ goes to 0 as $t \to \pm\infty$. In integrals over $-\infty \le x \le -A$ and $A \le x \le \infty$ we replace $u_{1,2}^{(\pm)}(x,k)$ by their asymptotics (2.36)-(2.39). Using estimates in Theorem 2.1, part (v), it is easy to show that for sufficiently large A the difference can be made arbitrarily small uniformly in t. To finish the proof it remains to show that for every continuous function $\varphi(k)$ on $(0, \infty)$ with compact support the integrals

$$J_1^{(\pm)}(t) = \frac{1}{2} \int_A^\infty \left| \int_0^\infty \varphi(k) e^{\mp ikx - ik^2 t} dk \right|^2 dx$$

and

$$J_2^{(\pm)}(t) = \frac{1}{2} \int_{-\infty}^A \left| \int_0^\infty \varphi(k) e^{\pm ikx - ik^2 t} dk \right|^2 dx$$

vanish as $t \to \pm\infty$. Consider, for instance, the integral $J_1^{(+)}(t)$. Given $\varepsilon > 0$, there exists a smooth function $\eta(k)$ on $(0, \infty)$ with compact support $[\alpha, \beta]$ such that

$$\|\varphi - \eta\|_{\mathscr{H}_0}^2 < \frac{\varepsilon}{4\pi}$$

We have by the Plancherel theorem,

$$J_1^{(+)}(t) = \frac{1}{2}\int_A^\infty \left|\int_0^\infty ((\varphi(k)-\eta(k))+\eta(k))e^{-ikx-ik^2t}dk\right|^2 dx$$
$$\le \int_A^\infty \left|\int_0^\infty (\varphi(k)-\eta(k))e^{-ikx-ik^2t}dk\right|^2 dx + \int_A^\infty \left|\int_0^\infty \eta(k)e^{-ikx-ik^2t}dk\right|^2 dx$$
$$\le \int_{-\infty}^\infty \left|\int_0^\infty (\varphi(k)-\eta(k))e^{-ikx-ik^2t}dk\right|^2 dx + \int_A^\infty \left|\int_0^\infty \eta(k)e^{-ikx-ik^2t}dk\right|^2 dx$$
$$\le \frac{\varepsilon}{2} + \int_A^\infty \left|\int_0^\infty \eta(k)e^{-ikx-ik^2t}dk\right|^2 dx.$$

To estimate the remaining integral we use integration by parts to obtain

$$\int_0^\infty \eta(k)e^{-i\left(kx+k^2t\right)}dk = \int_0^\infty \frac{\eta'(k)}{i(x+2kt)}e^{-i\left(kx+k^2t\right)}dk$$

and since $\frac{|\eta'(k)|}{x+2kt} \le \frac{C}{x+2\alpha t}$ for $x, t > 0$, we have

$$\int_A^\infty \left|\int_0^\infty \eta(k)e^{-i\left(kx+k^2t\right)}dk\right|^2 dx \le C^2\int_A^\infty \frac{dx}{(x+2\alpha t)^2} = \frac{C^2}{A+2\alpha t}$$

Choosing $t > \frac{2C^2}{\alpha\varepsilon}$, we obtain $J_1^{(+)}(t) < \varepsilon$. Other integrals are treated similarly.

Corollary 2.6. The wave operators satisfy orthogonality and completeness relations $W_\pm^* W_\pm = I$ and $W_\pm W_\pm^* = I - P$.

Proof. The result of Theorem 2.3, proved for the operator $\mathscr{U} = \mathscr{U}_-$, obviously holds for the operator $\mathscr{U}_+$. Thus relations (2.32) and (2.33) follow from the corresponding orthogonality and completeness relations for the operators $\mathscr{U}_\pm$.

Remark. The orthogonality relation (2.32) is trivial once the existence of the wave operators is established. Thus Theorem 2.5 gives another proof of the orthogonality relation in Theorem 2.3.

Problem 2.7 (The Cook's criterion). In abstract scattering theory, prove that the wave operators $W_\pm$exist if for all $\varphi \in \mathscr{H}$,

$$\int_0^\infty \left\|Ve^{-itH_0}\varphi\right\| dt < \infty.$$

Problem 2.8. Find the scattering matrix $S(k)$ for the potential $V(x)$ from Problem 2.5 and show that when $V_0 = 2\varkappa^2$, the scattering matrix is diagonal.

Problem 2.9 (Quantum tunneling). Find the scattering matrix $S(k)$ for the rectangular potential barrier: $V(x) = 0$ for $x < 0$ and $x > 2a$, and $V(x) = V_0 > 0$ for $0 \le x \le 2a$. Show that when E varies from 0 to V_0, T increases from 0 to $(1 + V_0a^2)^{-1}$ - the penetration of a potential barrier by a quantum particle.

2.4. Other boundary conditions.

Here we consider two examples of the Schrodinger operator

$$H = -\frac{d^2}{dx^2} + V(x)$$

with the potential $V(x)$ having different asymptotics as $x \to \pm\infty$.

Example 2.1. Suppose that the potential $V(x)$ satisfies

$$\int_{-\infty}^{0} (1+|x|)\left|V(x)-c^2\right| dx < \infty \quad \text{and} \quad \int_{0}^{\infty} (1+|x|)|V(x)|dx < \infty$$

for some $c > 0$. The Schrodinger operator H has negative discrete spectrum, consisting of finitely many simple eigenvalues $\lambda_1 < \cdots < \lambda_n < 0$, and absolutely continuous spectrum $[0, \infty)$, which is simple for $0 < \lambda < c^2$ and is of multiplicity two for $\lambda > c^2$. This qualitative structure of the spectrum is determined by the structure of the level sets $H_c(p, x) = \lambda$ of the classical Hamiltonian function $H_c(p, x) = p^2 + V(x)$: the eigenvalues could only appear for compact level sets, when the classical motion is periodic, while the values of λ with non-compact level sets, where the classical motion is
infinite, belong to the absolutely continuous spectrum. The absolutely continuous spectrum has multiplicity one or two depending on whether the corresponding classical motion is unbounded in one or in both directions, i.e., when $0 < \lambda < c^2$ or $\lambda > c^2$.

These results can be proved using methods in Section 2.1. Namely, set $\lambda = k^2$ and define the function $k_1 = \sqrt{k^2 - c^2}$ by the condition that $\operatorname{Im} k_1 \geq 0$ for $\operatorname{Im} k \geq 0$. In particular, $\operatorname{sgn} k_1 = \operatorname{sgn} k$ for k real, $|k| > c$. The differential equation

$$-y'' + V(x)y = k^2 y \tag{2.43}$$

for real k has two linear independent solutions $f_1(x, k), f_1(x, -k) = \overline{f_1(x, k)}$, where $f_1(x, k)$ has the asymptotics

$$f_1(x, k) = e^{ikx} + o(1) \quad \text{as} \quad x \to \infty.$$

For real $k, |k| > c$, equation (2.43) also has two linear independent solutions $f_2(x, k), f_2(x, -k) = \overline{f_2(x, -k)}$, where $f_2(x, k)$ has the asymptotics

$$f_2(x, k) = e^{-ik_1 x} + o(1) \quad \text{as} \quad x \to -\infty.$$

(Actually, these solutions satisfy estimates similar to that in Theorem 2.1.) As in Section 2.1, for real $k, |k| > c$, we have

$$f_2(x, k) = a(k)f_1(x, -k) + b(k)f_1(x, k),$$

where

$$a(k) = \frac{1}{2ik} W\left(f_1(x, k), f_2(x, k)\right), \quad b(k) = \frac{1}{2ik} W\left(f_2(x, k), f_1(x, -k)\right), \tag{2.44}$$

and $a(-k) = \overline{a(k)}, b(-k) = \overline{b(k)}$. However, $W\left(f_2(x, k), f_2(x, -k)\right) = -2ik_1$, so that for real $k, |k| > c$, we have

$$f_1(x, k) = \frac{k}{k_1} a(k) f_2(x, -k) - \frac{k}{k_1} b(-k) f_2(x, k).$$

From here we obtain the normalization condition

$$|a(k)|^2 - |b(k)|^2 = \frac{k_1}{k}, \quad |k| > c.$$

For fixed x solutions $f_1(x, k)$ and $f_2(x, k)$ can be analytically continued to the upper half-plane $\operatorname{Im} k > 0$. For $-c < k < c$ solution $f_2(x, k)$ is realvalued and satisfies

$$f_2(x, k) = a(k)f_1(x, -k) + \overline{a(k)f_1(x, -k)},$$

where $a(k)$ is still given by the same formula (2.44). The function $a(k)$ does not vanish for real k and admits meromorphic continuation to the upper half-plane $\operatorname{Im} k > 0$ where it has finitely many pure imaginary simple zeros $i\varkappa_1, ..., i\varkappa_n$ which correspond to the eigenvalues $\lambda_1 = -\varkappa_1^2, ..., \lambda_n = -\varkappa_n^2$.

The absolutely continuous spectrum of the Schrodinger operator H fills $[0, \infty)$. For $0 < \lambda = k^2 < c^2$ the spectrum is simple and

$$u(x, \lambda) = \frac{1}{a(k)} f_2(x, k), \quad 0 < k < c$$

are the corresponding normalized eigenfunctions of the continuous spectrum. For $\lambda = k^2 > c^2$ the spectrum has multiplicity two and

$$u_1(x, \lambda) = \frac{1}{a(k)} f_2(x, k), \quad u_2(x, k) = \frac{k_1}{ka(k)} f_1(x, k), \quad k > c$$

are the corresponding normalized eigenfunctions of the continuous spectrum. Denoting by $\psi_l(x)$ the normalized eigenfunctions of H corresponding to the eigenvalues λ_l, we get the eigenfunction expansion theorem: for $\psi \in L^2(\mathbb{R})$,

$$\psi(x) = \sum_{l=1}^{n} C_l \psi_l(x) + \int_0^c C(k) u(x, k) dk$$
$$+ \int_c^\infty \left(C_1(k) u_1(x, k) + C_2(k) u_2(x, k) \right) dk$$

where $C_l = (\psi, \psi_l), l = 1, ..., n$, and

$$C(k) = \int_{-\infty}^{\infty} \psi(x) \overline{u(x, k)} dx, \quad C_j(k) = \int_{-\infty}^{\infty} \psi(x) \overline{u_j(x, k)} dx, \quad j = 1, 2.$$

Example 2.2. Suppose that the potential $V(x)$ grows as $x \to -\infty$ and decays as $x \to \infty$:

$$\int_a^\infty (1 + |x|) |V(x)| dx < \infty \quad \text{for all} \quad a$$

and there exists $x_0 \in \mathbb{R}$ such that the spectrum of the Sturm-Liouville problem

$$-y'' + V(x) y = \lambda y, \quad -\infty < x \le x_0, \quad \text{and} \quad y'(x_0) = 0$$

is bounded below and discrete. The latter condition is a quantitative formulation of the property $\lim_{x \to -\infty} V(x) = \infty$.

Then for every real k there exists a solution $f(x, k)$ of the differential equation (2.43) with the asymptotics

$$f(x, k) = e^{ikx} + o(1) \quad \text{as} \quad x \to \infty$$

and there is a function $s(k)$ such that

$$u(x, k) = f(x, -k) + s(k) f(x, k)$$

is square integrable over $(-\infty, a)$ for any real a. The Schrodinger operator H has simple absolutely continuous spectrum $[0, \infty)$ and discrete spectrum consisting of finitely many negative eigenvalues. Functions $u(x, k)$ are normalized eigenfunctions of the continuous spectrum and the corresponding eigenfunction expansion theorem has the following form: for every $\psi \in L^2(\mathbb{R})$,

$$\psi(x) = \sum_{l=1}^{n} C_l \psi_l(x) + \int_0^\infty C(k) u(x,k) dk$$

where $C_l = (\psi, \psi_l), l = 1, ..., n$, and

$$C(k) = \int_{-\infty}^{\infty} \psi(x) \overline{u(x,k)} dx$$

Problem 2.10. Give an explicit form of the eigenfunction expansion theorem for the potential $V(x) = e^x$.

Problem 2.11. Find energy levels for the Morse potential $V(x) = e^{-2\alpha x} - 2e^{-\alpha x}$, $\alpha > 0$.

Problem 2.12. Give an explicit form of the eigenfunction expansion theorem for the potential $V(x) = Fx$, describing the motion of a quantum particle in a homogeneous field; according to Problem 1.4, the corresponding Schrodinger operator is self-adjoint. (Hint: Solve the Schrodinger equation explicitly in the momentum representation, and express normalized eigenfunctions of the continuous spectrum in the coordinate representation in terms of Airy-Fock functions, defined in Section 6.2.)

Problem 2.13. Give an explicit form of the eigenfunction expansion theorem for the potential $V(x) = -\frac{1}{2}kx^2$, where $k > 0$ (according to Problem 1.4, the corresponding Schrodinger operator is self-adjoint).

3.6.6 One-Dimensional Schrödinger Equation 3: Basic Examples

Одномерный ящик с бесконечными стенками (?)

Найдем уровни энергии в *одномерном ящике*, то в: $V(x) = \begin{cases} 0, & 0 < x < a \\ \infty, & x < 0, x > a \end{cases}$

Волновую функцию находим, решая уравнение Шредингера с граничными условиями, энергию находим с помощью k, который квантуется из вида волновой функции и граничных условий.

Уравнение Шредингера есть:

$$\psi'' + \frac{2m}{h^2}(E - U(x))\psi(x) = 0$$

Введем $k^2 = \frac{2mE}{\hbar^2}$, внутри ямы:

$$\psi'' + k^2\psi(x) = 0,$$

Общее решение $\psi(x) = c_1 e^{ikx} + c_2 e^{-ikx}$, и при граничных условиях $\psi(0) = \psi(a) = 0$ дает:

$$\psi(x) = C_1 \sin(kx), \quad ka = \pi n, \quad n \in \mathbb{N},$$
$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2ma^2}.$$

и в итоге учетом нормировки волновая функция имеет вид:

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin \frac{\pi n}{a} x, & 0 < x < a \\ 0, & x \leqslant 0, x \geqslant a \end{cases}$$

Заметим также, что на границах имеется скачек производной.

Посмотрим на свойства наших решений. Посчитаем дисперсию:

$$\langle x\rangle = \int\limits_0^a dx\psi^2(x)x = \frac{a}{2},$$

$$\left\langle x^2\right\rangle = \int\limits_0^a dx\psi^2(x)x^2 = \frac{a^2}{3} - \frac{a^2}{2\pi^2 n^2}$$

$$(\Delta x)^2 = \frac{a^2}{12}\left(1 - \frac{6}{\pi^2 n^2}\right)$$

Для импульса:

$$(\Delta p)^2 = \left\langle p^2\right\rangle = \langle 2mE_n\rangle = \frac{\hbar^2}{a^2}\pi^2 n^2.$$

Сравним с классическим случаем, в котором распределение равномерное, то есть $\rho(x) = 1/a$:

$$\overline{x} = \int\limits_0^a x\rho(x) = \frac{a}{2}, \quad \overline{(\Delta\hat{x})^2} = \frac{a^2}{12}$$

Видим, что в квантовом случае дисперсия другая.
(???? как так??)
Теперь можно посчитать фазовый объем. Заметим, что для любого n

$$(\Delta x)^2(\Delta p)^2 = \frac{\hbar^2}{12}\left(\pi^2 n^2 - 6\right) \geqslant \frac{\hbar^2}{4},$$

поэтому ячейка фазового пространства для одного состояния имеет

$$\Delta\Gamma|_{\Delta n=1} = \frac{d\Delta\Gamma}{dn}\Delta n \to \frac{\hbar}{2\sqrt{3}}\pi.$$

(? зачем эта ячейка? потом вернусь, отвечу, если буду понимать.)
(какие еще выводы есть???)
Волновая функция частицы в импульсном представлении:

$$\psi_n(p) \equiv \langle p|n\rangle = \int\limits_0^1 \langle p|x\rangle\langle x|n\rangle dx = \int\limits_0^1 \frac{1}{\sqrt{2\pi}}e^{-ipx}\sqrt{2}\sin n\pi x dx = -i2\sqrt{\pi}\mathrm{e}^{-i\frac{(p-n\pi)}{2}}\frac{n\sin\left(\frac{p-n\pi}{2}\right)}{p^2-(n\pi)^2}.$$

В квазиклассическом приближении ($n \gg 1$) распределение по импульсам вблизи $p = \pm n\pi$ имеет вид

$$|\psi_n(p)|^2 \simeq \frac{\sin^2(\varepsilon/2)}{\pi\varepsilon^2}, \quad \int\limits_{-\infty}^{\infty}\frac{\sin^2(\varepsilon/2)}{\pi\varepsilon^2}d\varepsilon = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty}\frac{\sin^2 x}{x^2}dx = \frac{1}{2},$$

где $\varepsilon = p \pm n\pi$, что соответствует классической плотности вероятности распределения по импульсам:

$$\rho(p) = \frac{1}{2}\delta\left(p - p_n\right) + \frac{1}{2}\delta\left(p + p_n\right), \quad p_n = \sqrt{2E_n} = \pi n.$$

Фазовая плоскость, как и траектория частицы на ней, - понятие классическое, поэтому рассмотрим эту часть задачи в квазиклассическом приближении: $\hbar \to 0, n \to \infty$ при конечном hn. Фазовые объёмы для состояний с энергией $E \leqslant E_n$ и $E \leqslant E_{n+1}$ имеют вид

$$\Gamma_n = 2p_n a = 2\pi hn \quad \left(p_n = \sqrt{2mE_n} = \frac{\pi\hbar}{a}n\right),$$

$$\Gamma_{n+1} = 2p_{n+1}a = 2\pi h(n+1)$$

Следовательно, объём, приходящийся на одно квантовое состояние,

$$\Delta\Gamma_n = \Gamma_{n+1} - \Gamma_n = 2\pi\hbar.$$

Мелкая яма

Обсудим подробно мелкую яму.

Описание мелкой ямы

Критерии существования основного состояния в мелкой яме

Основное состояние в мелкой яме единственное

(подробно про этот факт, и запоминаем его.)

О моделях из дельта-потенциалов

(укажу потом методы для них и их применения, пока об этом в каталоге задач.)

Особенности моделей из дельта-потенциалов (??)

О применениях (??)

(эта модель применяется дальше или все на неё забили? если да - укажу в части ниже, где и как.)

О других типичных одномерных ямах

(по идее тут заготовка к задачам овчинкина)

Если есть возможность - интегралы считаем на компьютере

Потом уже руками. Так в разы быстрее и меньше вероятности ошибок. А тут очень часто можно фигню насчитать.

Theory from Landau

Вообще говоря, до сих пор мы обсуждали стационарные задачи.

С другой стороны, с точки зрения задачи рассеяния более логичной кажется задача нестационарная, для определения которой нам необходимо:

1.

Задать начальные условия, которые соответствуют волновому пакету, находящемуся на $x \to -\infty$ при времени $\tau \to -\infty$ и имеющему конечный импульс p_0, направленный на рассеиватель.

Примером такого волнового пакета может служить следующая волновая функция:

$$\psi\left(x, -\tau_0\right) \equiv \psi_0(x) = \frac{1}{\pi^{1/4} a^{1/2}} \exp\left(-\frac{(x+L)^2}{2a^2} + ip_0 x\right)$$

В координатном представлении она представляет собой волновой пакет ширины a вокруг точки $x = -L$, а в импульсном - волновой пакет ширины $\sim 1/a$ вокруг среднего значения k_0

2. Решить нестациониое уравнение Шрёдингера, рассмотрев эволюцию этого волнового пакета.

3. Исследовать асимптотики полученного решения при $\tau \to +\infty$, которые представляли бы пару волновых пакетов отражённый, который находится на $x \to -\infty$ и имеет импульс $-p$, и прошедший, который летит на $x \to +\infty$ и имеет импульс p

4. Наконец, вычислить вероятность отражения $R = \int\limits_{\infty}^{0} |\psi(x, \tau \to +\infty)|^2 dx$ и $T = \int\limits_{0}^{\infty} |\psi(x, \tau \to +\infty)|^2 dx$ Априори утверждение о том, что эти вероятности совпадают с вероятностями, которые мы определили в стационарной задаче рассеяния, не является очевидным.

Тем не менее, это действительно так, что мы попробуем продемонстрировать ниже, для чего мы попробуем решить нестационарное уравнение Шрёдингера в общем виде. ивателя не было, то волновой пакет тоже имелся бы, но двигался бы он правее.

Явление это носит название задержки

волнового пакета - частица может на некоторое время кзастрять в рассеивателезз.

Мы ставим своей целью найти время этой задержки.

Для решения нестационарного УШ, как обычно, необходимо разложиться по базису стационарных решений (3.32), для чего мы можем воспользоваться выведенной выше нормировкой состояний непрерывного спектра [24]:

$$\hat{\mathbb{I}} = \int\limits_{0}^{\infty} \frac{dp}{2\pi} \left(\left|\psi_p^{(+)}\right\rangle \left\langle \psi_p^{(+)}\right| + \left|\psi_p^{(-)}\right\rangle \left\langle \psi_p^{(-)}\right| \right)$$

Разложимся по базису, используя асимптотики при $x \to -\infty$

$$\psi_+(p) = \left\langle \psi_p^{(+)} | \psi_0 \right\rangle = 2^{1/2}\pi^{1/4}a^{1/2} \left[\exp\left(-\frac{1}{2}(p-p_0)^2 a^2 + i(p-p_0)L \right) + \right.$$
$$\left. + \, r^* \exp\left(-\frac{1}{2}(p+p_0)^2 a^2 - i(p+p_0)L \right) \right]^0$$

Из физической интуиции понятно, что нас интересует именно первый член, ведь он возник из асимптотики падающей волны в задаче рассеяния.

Математически же это соответствует тому, что интегрируем мы по импульсам $p > 0$, а p_0 -большой положительный импульс, поэтому второй вклад оказывается экспоненциально малым.

Ровно по этой же причине, коэффициенты разложения по $\left|\psi_p^{(-)}\right\rangle$, как и следует из нашей физической интуиции (ведь это - решение задачи рассеяния ксправа-налевож!) тоже будут экспоненциально малы и нас интересовать не будут.

Дальше мы должны решать нестационарное уравнение Шрёдингера.

Поскольку $\left|\psi_p^{(+)}\right\rangle$ эволюционируют тривиальным образом, накручивая фазу $e^{-i\varepsilon_p\tau}$, то $\psi_+(p,t) = e^{-i\varepsilon_p\tau}\psi_+(p)$. Наконец, мы должны сделать кобратное преобразование Фурье и записать:

$$\psi(x,\tau) = \int \frac{dp}{2\pi} \psi_+(p,\tau) \cdot \psi_p^{(+)}(x) =$$
$$= 2^{1/2}\pi^{1/4}a^{1/2} \int \frac{dp}{2\pi} \psi_p^{(+)}(x) \exp\left(-\frac{1}{2}(p-p_0)^2 a^2 + i(p-p_0)L \right) e^{-i\varepsilon_p(\tau+\tau_0)}$$

Мы не знаем явный вид функции $\psi_p^{(+)}(x)$, но знаем асимптотики при $x \to \pm\infty$, поэтому давайте посмотрим на асимптотики $\psi(x,\tau)$ при $x \to \pm\infty$. При этом интеграл имеет пик

вблизи $p = p_0$, поэтому все величины мы разложим вблизи этой точки и возьмём интеграл методом перевала.

При этом учтём, что амплитуды прохождения, вообще говоря, тоже зависят от импульсов, и их тоже стоит раскладывать: $t \equiv t(p) = \sqrt{T(p)}e^{i\theta_p}$. Именно из-за зависимости фазы от импульса и произойдёт в конечном итоге эффект задержки.

Итак, раскладываем ε_p и θ_p до второго порядка и берем Гауссов интеграл:

Мы не знаем явный вид функции $\psi_p^{(+)}(x)$, но знаем асимптотики при $x \to \pm\infty$, поэтому давайте посмотрим на асимптотики $\psi(x,\tau)$ при $x \to \pm\infty$. При этом интеграл имеет пик вблизи $p = p_0$, поэтому все величины мы разложим вблизи этой точки и возьмём интеграл методом перевала.

При этом учтём, что амплитуды прохождения, вообще говоря, тоже зависят от импульсов, и их тоже стоит раскладывать: $t \equiv t(p) = \sqrt{T(p)}e^{i\theta_p}$. Именно из-за зависимости фазы от импульса и произойдёт в конечном итоге эффект задержки.

Итак, раскладываем ε_p и θ_p до второго порядка и берем Гауссов интеграл:

$$\psi(x \to +\infty, \tau) \approx 2^{1/2}\pi^{1/4}a^{1/2}\int \frac{dp}{2\pi}\sqrt{T(k)}\exp\left(i\left[\theta_{p_0} + \theta'_{p_0}(p-p_0) + \frac{1}{2}\theta''_{p_0}(p-p_0)^2\right]\right)\cdot e^{ipx}$$
$$\cdot\exp\left(-\frac{1}{2}(p-p_0)^2 a^2 + i(p-p_0)L\right)\cdot\exp\left(-i\left[\varepsilon_{p_0} + \varepsilon'_{p_0}(p-p_0) + \frac{1}{2}\varepsilon''_{p_0}(p-p_0)^2\right](\tau+\tau_0)\right) =$$
$$= \frac{a^{1/2}}{\pi^{1/4}\widetilde{a}(t)}\sqrt{T(p_0)}\exp\left[-\frac{[(x+L)+\theta'(p_0)-\varepsilon'(p_0)(\tau+\tau_0)]^2}{2\widetilde{a}^2(t)} + i\cdot\text{ phase }\right]$$

где $\widetilde{a}^2(t) = a^2 - i\theta''(p_0) + i\varepsilon''(p_0)(\tau+\tau_0)$. Исследуем теперь полученное выражение:

1.

Это - гауссов волновой пакет, центр которого расположен при $x_0(\tau) = -L - \theta'(p_0) + \varepsilon'(p_0)(\tau+\tau_0) = -L + \varepsilon'(p_0)(\tau + \tau_0 - \theta'/\varepsilon')$.

Это соответствует пакету, который движется с групповой скоростью $v = \partial\varepsilon/\partial p = p/m$. Однако выражение это устроено так, будто он стартовал из точки $-L$ не в момент времени $\tau = -\tau_0$ (как было бы со свободным движением), а чуть позже, в момент времени $\tau = -\tau_0 + \theta'/\varepsilon'$. Это и есть явление задержки волнового пакета; время же задержки равно $|\Delta\tau = \theta'/\varepsilon' = \partial\theta/\partial\varepsilon$. Тут сразу же возникает важнейшее свойство фазы – ведь в силу причинности, $\Delta\tau > 0$ (частица не может прилететь к детектору раньше, чем если бы она летела баллистически!) а значит, фаза рассеяния является монотонной функцией энергии.

2.

Ширина этого пакета определяется из условия $\frac{1}{a^2(t)} = \mathrm{Re}\,\frac{1}{\widetilde{a}^2(t)} \to a^2(t) = a^2 + \frac{[\varepsilon''(p_0)(\tau+\tau_0)-\theta''(p_0)]^2}{a^2}$.

Этот эффект называется расплыванием волнового пакетаж, и связан он с наличием у спектра кривизны $^{25}\varepsilon''(p_0)$; из-за соотношения неопределённостей, в пакет всегда будут входить частицы со слегка разными импульсами, а значит - и с разными скоростями.

Поэтому со временем ширина пакета будет меняться.

3. Наконец, полное число частиц в этом пакете равно $\int\limits_{-\infty}^{\infty}|\psi(x \to +\infty, \tau)|^2 dx = T(p_0)$ - что и завершает связь стационарной и нестационарной задачи рассеяния.

Исследование асимптотики $\psi(x \to -\infty, \tau)$ проходит абсолютно аналогично -вклад при этом будет приходить от котражённой волныж re^{-ipx}, а вклад от кпадающей e^{ipx} будет экспоненциально маленьким.

3.6.7 Schrodinger Equation in a Rotated Frame

(read articles about it, I don't know yet)

3.6.8 Experimental Confirmation of Schrodinger Equation

(I'll collect some experiments here)

Догадка про УШ из эксперимента

как?

3.6.9 3. Angular momentum and SO(3)

3.1. Angular momentum operators.

In Chapter 1 (see Example 1.10 in Section 1.4) for a classical particle in $\mathbb{R}^3$ we introduced the angular momentum vector $\boldsymbol{M}_{\mathrm{c}} = \boldsymbol{x} \times \boldsymbol{p}$ with components

$$M_{\mathrm{c}1} = x_2p_3 - x_3p_2, \quad M_{\mathrm{c}2} = x_3p_1 - x_1p_3, \quad M_{\mathrm{c}3} = x_1p_2 - x_2p_1$$

According to Example 2.1 in Section 2.6 of Chapter 1, they have the following Poisson brackets with respect to the canonical Poisson structure on $T^*\mathbb{R}^3$:

(3.1) $\{M_{\mathrm{c}1}, M_{\mathrm{c}2}\} = -M_{\mathrm{c}3}, \quad \{M_{\mathrm{c}2}, M_{\mathrm{c}3}\} = -M_{\mathrm{c}1}, \quad \{M_{\mathrm{c}3}, M_{\mathrm{c}1}\} = -M_{\mathrm{c}2}.$

The square of the angular momentum $\boldsymbol{M}_{\mathrm{c}}^2 = M_{\mathrm{c}1}^2 + M_{\mathrm{c}2}^2 + M_{\mathrm{c}3}^2$ satisfies

$$\left\{\boldsymbol{M}_{\mathrm{c}}^2, M_{\mathrm{c}1}\right\} = \left\{\boldsymbol{M}_{\mathrm{c}}^2, M_{\mathrm{c}2}\right\} = \left\{\boldsymbol{M}_{\mathrm{c}}^2, M_{\mathrm{c}3}\right\} = 0$$

If the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{x}) = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{x})$$

is invariant under rotations, $V(\boldsymbol{x}) = V(|\boldsymbol{x}|)$, then components of the angular momentum are the integrals of motion

$$\{H_{\mathrm{c}}, M_{\mathrm{c}1}\} = \{H_{\mathrm{c}}, M_{\mathrm{c}2}\} = \{H_{\mathrm{c}}, M_{\mathrm{c}3}\} = 0 \quad \text{and} \quad \left\{H_{\mathrm{c}}, M_{\mathrm{c}}^2\right\} = 0$$

This can also be verified directly using Poisson brackets

$$\{M_{\mathrm{c}j}, p_k\} = -\varepsilon_{jkl}p_l \quad \text{and} \quad \{M_{\mathrm{c}j}, x_k\} = -\varepsilon_{jkl}x_l, \quad i, j, k = 1, 2, 3 \tag{3.2}$$

where ε_{jkl} is a totally anti-symmetric tensor, $\varepsilon_{123} = 1$.

Correspondingly, in quantum mechanics the components of the angular momentum operator $\boldsymbol{M} = \boldsymbol{Q} \times \boldsymbol{P}$ are defined by

$$M_1 = Q_2P_3 - Q_3P_2, \quad M_2 = Q_3P_1 - Q_1P_3, \quad M_3 = Q_2P_3 - Q_3P_2$$

where $\boldsymbol{Q} = (Q_1, Q_2, Q_3)$ and $\boldsymbol{P} = (P_1, P_2, P_3)$ are, respectively, coordinate and momentum operators. Since operators Q_i and P_k commute for $i \neq k$, there is no ordering problem when defining quantum angular momentum operators. It follows from Heisenberg commutation relations that their quantum brackets are the same as the corresponding Poisson brackets (3.1):

$$\{M_1, M_2\}_\hbar = -M_3, \quad \{M_2, M_3\}_\hbar = -M_1, \quad \{M_3, M_1\}_\hbar = -M_2 \tag{3.3}$$

Equivalently,

$$[M_1, M_2] = i\hbar M_3, \quad [M_2, M_3] = i\hbar M_1, \quad [M_3, M_1] = i\hbar M_2 \tag{3.4}$$

The operator of the square of the total angular momentum $\boldsymbol{M}^2 = M_1^2 + M_2^2 + M_3^2$ satisfies

$$\left[\boldsymbol{M}^2, M_1\right] = \left[\boldsymbol{M}^2, M_2\right] = \left[\boldsymbol{M}^2, M_3\right] = 0$$

Correspondingly, for the Hamiltonian operator

$$H = \frac{\boldsymbol{P}^2}{2m} + V(\boldsymbol{Q})$$

with spherically symmetric potential $V(\boldsymbol{x}) = V(|\boldsymbol{x}|)$ operators M_1, M_2, M_3 and, therefore, $\boldsymbol{M}^2$, are quantum integrals of motion:

$$[H, M_1] = [H, M_2] = [H, M_3] = 0 \quad \text{and} \quad \left[H, M^2\right] = 0$$

This can be verified directly by using quantum brackets

$$\{M_j, P_k\}_\hbar = -\varepsilon_{jkl} P_l, \quad \{M_j, Q_k\}_\hbar = -\varepsilon_{jkl} Q_l, \quad j,k,l = 1,2,3 \tag{3.5}$$

which are the same as Poisson brackets (3.2), and follow from Heisenberg commutation relations.

In the coordinate representation $\mathscr{H} = L^2\left(\mathbb{R}^3, d^3\boldsymbol{x}\right)$ the operators of angular momentum are given by the following first order self-adjoint differential operators:

$$M_1 = i\hbar\left(x_3\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_3}\right) \tag{3.6}$$

$$M_2 = i\hbar\left(x_1\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_1}\right) \tag{3.7}$$

$$M_3 = i\hbar\left(x_2\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_2}\right) \tag{3.8}$$

They have the property that

$$M_1\psi = M_2\psi = M_3\psi = 0$$

for any spherically symmetric smooth function $\psi(\boldsymbol{x}) = \psi(|\boldsymbol{x}|)$. In other words, angular momentum operators act only on the angle coordinates in $\mathbb{R}^3$. Namely, let

$$x_1 = r\sin\vartheta\cos\varphi, \quad x_2 = r\sin\vartheta\sin\varphi, \quad x_3 = r\cos\vartheta,$$

where $0 \le \vartheta < \pi, 0 \le \varphi < 2\pi$, be the spherical coordinates in $\mathbb{R}^3$. Explicit computation gives

$$M_1 = i\hbar\left(\sin\varphi\frac{\partial}{\partial\vartheta} + \cot\vartheta\cos\varphi\frac{\partial}{\partial\varphi}\right)$$

$$M_2 = -i\hbar\left(\cos\varphi\frac{\partial}{\partial\vartheta} - \cot\vartheta\sin\varphi\frac{\partial}{\partial\varphi}\right)$$

$$M_3 = -i\hbar\frac{\partial}{\partial\varphi}$$

Thus

$$\boldsymbol{M}^2 = -\hbar^2\left(\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right),$$

so that the operator $-\frac{1}{\hbar^2}\boldsymbol{M}^2$ is the spherical part of the Laplace operator in $\mathbb{R}^3$,

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}\boldsymbol{M}^2 \tag{3.9}$$

3.2. Representation theory of SO(3). Quantum operators of angular momentum are related with the representation theory of the rotation group SO(3) - the group of 3×3 orthogonal matrices with determinant 1.SO(3) is a compact Lie group, isomorphic to the real projective space $\mathbb{RP}^3$ as a smooth manifold. There is a Lie group isomorphism $\mathrm{SO}(3)\simeq \mathrm{SU}(2)/\{\pm I\}$, where SU(2) is a Lie group of 2×2 unitary matrices with determinant 1 .

The Lie algebra $\mathfrak{so}(3)$ of SO(3) is a three-dimensional Lie algebra of 3×3 skew-symmetric matrices, with the basis

$$X_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad X_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad X_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The matrices X_1, X_2, X_3 correspond, respectively, to the one-parameter subgroups of SO(3) consisting of rotations about coordinate axes in $\mathbb{R}^3$. They satisfy commutation relations

$$[X_1, X_2] = X_3, \quad [X_2, X_3] = X_1, \quad [X_3, X_1] = X_2$$

which are similar to (3.4). To establish the connection between quantum angular momentum operators and representation theory of SO(3), consider the regular representation R of SO(3) in $\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{x})$, defined by

$$(R(g)\psi)(\boldsymbol{x}) = \psi\left(g^{-1}\boldsymbol{x}\right), \quad g\in \mathrm{SO}(3), \psi\in\mathscr{H}$$

Lemma 3.1. We have

$$R\left(e^{u_1X_1+u_2X_2+u_3X_3}\right) = e^{-\frac{i}{\hbar}(u_1M_1+u_2M_2+u_3M_3)}.$$

Proof. Put $\boldsymbol{uX} = u_1X_1+u_2X_2+u_3X_3$ and $\boldsymbol{uM} = u_1M_1+u_2M_2+u_3M_3$. It follows from the Stone theorem and direct computation that

$$i\hbar\frac{\partial}{\partial u_j}\bigg|_{\boldsymbol{u}=0} R\left(e^{\boldsymbol{uX}}\right) = M_j, \quad j=1,2,3$$

where self-adjoint operators M_1, M_2, M_3 are given by (3.6)-(3.8). Next, for fixed u_1, u_2, u_3, consider the following one-parameter group $U(t) = R\left(e^{t\boldsymbol{uX}}\right)$ of unitary operators in $\mathscr{H}$. By the Stone theorem, $U(t) = e^{-itA}$, where

$$A = i\frac{d}{dt}\bigg|_{t=0} U(t) = \frac{1}{\hbar}\boldsymbol{uM}$$

Remark. We have $M_j = i\hbar\rho(X_j)$, where $\rho = dR$ is the corresponding regular representation of the Lie algebra $\mathfrak{so}(3)$ in $\mathscr{H}$.

All irreducible unitary representations R_l of the Lie group SO(3) are finite-dimensional and are parametrized by non-negative integers $l\geq 0$. The corresponding irreducible representation $\rho_l = dR_l$ of the Lie algebra $\mathfrak{so}(3)$ in $2l+1$-dimensional complex vector space V_l can be explicitly described as follows. Introduce Hermitian operators $T_j = i\rho_l(X_j), j=1,2,3$, which satisfy commutation relations

$$[T_1, T_2] = iT_3, \quad [T_3, T_1] = iT_2, \quad [T_2, T_3] = iT_1$$

The vector space V_l has an orthonormal basis $\{e_{lm}\}_{m=-l}^{m=l}$ such that

$$(T_1 - iT_2)\, e_{lm} = -\sqrt{(l+m)(l-m+1)}e_{lm-1}, \tag{3.10}$$

$$(T_1 + iT_2)\, e_{lm} = -\sqrt{(l-m)(l+m+1)}e_{lm+1}, \tag{3.11}$$

$$T_3 e_{lm} = m e_{lm} \tag{3.12}$$

In particular, $(T_1 + iT_2)\, e_{ll} = 0$, so that V_l is the highest weight module. The representation ρ_l is irreducible, and we have by Schur's lemma

$$\boldsymbol{T}^2 = l(l+1)I_l,$$

where I_l is the identity operator in V_l. This can also be verified directly by using (3.10)-(3.12).

Remark. When l is a half-integer, i.e., $l \in \frac{1}{2} + \mathbb{Z}_{\geq 0}$, and $m = -l, -l+1, ..., l-1, l$, formulas (3.10)-(3.12) still define an irreducible highest weight representation ρ_l of the Lie algebra $\mathfrak{so}(3)$ of dimension $2l+1$, and every irreducible n-dimensional representation of $\mathfrak{so}(3)$ is isomorphic to the representation ρ_l with $l = \frac{n-1}{2}$. For half-integer l, representations ρ_l are not integrable: they give rise to two-valued representations of SO(3), the socalled spinor representations. However, considered as representations of the Lie algebra $\mathfrak{su}(2) \simeq \mathfrak{so}(3)$, ρ_l correspond to the irreducible unitary representations of the Lie group SU(2). It follows from the representation theory of SU(2) that for $l, l' \in \frac{1}{2}\mathbb{Z}_{\geq 0}$,

$$V_l \otimes V_{l'} = \bigoplus_{j=|l-l'|}^{l+l'} V_j, \tag{3.13}$$

the so-called Clebsch-Gordan decomposition. In physics, it corresponds to the addition of angular momenta.

The regular representation R of SO(3) in $\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{x})$ is not irreducible. We have

$$\mathscr{H} = L^2\left(S^2, d\boldsymbol{n}\right) \otimes L^2\left(\mathbb{R}_{>0}, r^2 dr\right), \tag{3.14}$$

where $d\boldsymbol{n}$ is the measure on S^2 induced by the Lebesgue measure on $\mathbb{R}^3$. The group SO(3) acts by rotations in the first factor of the tensor product (3.14), whereas in the second factor it acts as the identity operator. Thus the problem of decomposing the regular representation R reduces to finding SO(3) invariant subspaces of the Hilbert space $L^2(S^2, d\boldsymbol{n})$. The result is the orthogonal sum decomposition

$$L^2\left(S^2, d\boldsymbol{n}\right) = \bigoplus_{l=0}^{\infty} \mathscr{D}_l, \tag{3.15}$$

where $\mathscr{D}_l \simeq V_l$. Under this isomorphism, the orthonormal basis Y_{lm} in $\mathscr{D}_l$ which corresponds to the basis e_{lm} in V_l is given by the normalized spherical functions

$$Y_{lm}(\vartheta, \varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} P_l^m(\cos\vartheta), \quad m = -l, ..., l$$

where $P_l^m(x)$ are normalized associated Legendre polynomials,
$P_l^m(x) = (-1)^m \sqrt{\frac{(l+m)!}{(l-m)!}} \sqrt{\frac{2l+1}{2}} \frac{1}{2^l l!} (1-x^2)^{-\frac{m}{2}} \frac{d^{l-m}}{dx^{l-m}} (x^2-1)^l, \quad |x| < 1.$
The self-adjoint operator $\boldsymbol{M}^2$ in the Hilbert space $L^2(S^2, d\boldsymbol{n})$ has pure point spectrum consisting of eigenvalues $\hbar^2 l(l+1)$ of multiplicities $2l+1$, $l = 0, 1, 2, ...$, and the decomposition (3.15) gives its eigenfunction expansion: for every $\psi \in L^2(S^2, d\boldsymbol{n})$,
$\psi = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} C_{lm} Y_{lm}$, where $C_{lm} = \int_0^{2\pi} \int_0^{\pi} \psi(\vartheta, \varphi) \overline{Y_{lm}(\vartheta, \varphi)} \sin\vartheta d\vartheta d\varphi$.

Problem 3.

1. Prove all results in this section. (Hint: See the list of references to this chapter.)

3.6.10 4. Two-body problem

(???? are there are really answer here about two-body problem in QM?)

4.1. Separation of the center of mass.

Consider the Schrodinger operator for the two-body problem (see Example 2.2 in Section 2.4 in Chapter 2)

$$H = -\frac{\hbar^2}{2m_1}\Delta_1 - \frac{\hbar^2}{2m_2}\Delta_2 + V(\boldsymbol{x}_1 - \boldsymbol{x}_2)$$

Introducing

$$\boldsymbol{X} = \frac{m_1\boldsymbol{x}_1 + m_2\boldsymbol{x}_2}{m_1 + m_2} \quad \text{and} \quad \boldsymbol{x} = \boldsymbol{x}_1 - \boldsymbol{x}_2$$

the coordinate of the center of mass and the relative coordinate, we get

$$H = -\frac{\hbar^2}{2M}\Delta_{\boldsymbol{X}} - \frac{\hbar^2}{2\mu}\Delta_{\boldsymbol{x}} + V(\boldsymbol{x})$$

where $M = m_1 + m_2$ is the total mass and $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is the reduced mass. The Hamiltonian operator H can be diagonalized by the method of separation of variables. Namely, consider the following decomposition of the two-body Hilbert space $\mathscr{H} = L^2(\mathbb{R}^6)$ into the tensor product of Hilbert spaces:

$$\mathscr{H} = L^2\left(\mathbb{R}^3, d^3\boldsymbol{X}\right) \otimes L^2\left(\mathbb{R}^3, d^3\boldsymbol{x}\right) \tag{4.1}$$

The operator

$$H_{\boldsymbol{X}} = -\frac{\hbar^2}{2M}\Delta_{\boldsymbol{X}} \tag{4.2}$$

acts as the identity operator in the second factor of (4.1), and the operator

$$H_{\boldsymbol{x}} = -\frac{\hbar^2}{2\mu}\Delta_{\boldsymbol{x}} + V(\boldsymbol{x}) \tag{4.3}$$

acts as the identity operator in the first factor of (4.1). For the solutions of the eigenvalue problem

$$H\psi = E\psi \tag{4.4}$$

in the product form

$$\psi(\boldsymbol{X}, \boldsymbol{x}) = \Psi(\boldsymbol{X})\psi(\boldsymbol{x}),$$

the variables are separated:

$$H_{\boldsymbol{X}}\Psi(\boldsymbol{X}) = E_1\Psi(\boldsymbol{X}) \quad \text{and} \quad H_{\boldsymbol{x}}\psi(\boldsymbol{x}) = E_2\psi(\boldsymbol{x}),$$

where $E = E_1 + E_2$. Since

$$\Psi(\boldsymbol{X}) = \left(\frac{1}{2\pi\hbar}\right)^{\frac{3}{2}} e^{\frac{i}{\hbar}\boldsymbol{kX}}, \quad \boldsymbol{k}^2 = 2ME_{\mathbf{1}}$$

the quantum two-body problem reduces to the problem of a quantum particle moving in the potential field, and is described by the Hamiltonian operator (4.3) in the Hilbert space $L^2(\mathbb{R}^3, d^3\boldsymbol{x})$.

4.2. Three-dimensional scattering theory.

Here we outline the scattering theory for the Schrodinger operator $H = -\Delta + V(\boldsymbol{x})$ (where we put $\hbar = 1$ and $\mu = \frac{1}{2}$) with rapidly decreasing potential. Specifically, assume that the bounded, real-valued function $V(\boldsymbol{x})$ on $\mathbb{R}^3$ satisfies

$$V(\boldsymbol{x}) = O\left(|\boldsymbol{x}|^{-3-\varepsilon}\right) \quad \text{as} \quad |\boldsymbol{x}| \to \infty \tag{4.5}$$

for some $\varepsilon > 0$. Then for every $k \in \mathbb{R}^3$ the Schrodinger equation

$$-\Delta\psi(\boldsymbol{x}) + V(\boldsymbol{x})\psi(\boldsymbol{x}) = k^2\psi(\boldsymbol{x}), \quad k = |\boldsymbol{k}|, \tag{4.6}$$

has two solutions $u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})$ satisfying the following asymptotics as $|\boldsymbol{x}| \to \infty$:

$$u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k}) = e^{i\boldsymbol{kx}} + f^{(\pm)}(k, \boldsymbol{\omega}, \boldsymbol{n})\frac{e^{\pm ikr}}{r} + o\left(\frac{1}{r}\right) \tag{4.7}$$

where $\boldsymbol{k} = k\boldsymbol{\omega}, \boldsymbol{x} = r\boldsymbol{n}$. Asymptotics (4.7) are called Sommerfeld's radiation conditions. To prove the existence of solutions $u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})$, one should consider the following integral equations:

$$u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k}) = c^{i\boldsymbol{kx}} + \int_{\mathbb{R}^3} G^{(\pm)}(\boldsymbol{x} - \boldsymbol{y}, k)V(\boldsymbol{y})u^{(\pm)}(\boldsymbol{y}, \boldsymbol{k})d^3\boldsymbol{y} \tag{4.8}$$

where

$$G^{(\pm)}(\boldsymbol{x}, k) = -\frac{1}{4\pi}\frac{e^{\pm ikr}}{r}.$$

Integral equations (4.8) are equivalent to the Schrodinger equation (4.6) with Sommerfeld's radiation conditions (4.7), and are called Lippman-Schwinger equations. Their analysis uses Fredholm theory and Kato's Theorem 1.8.

Solutions $u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})$ are called stationary scattering waves. They are analogous to the solutions $u_j^{(\pm)}(x, k)$ for the one-dimensional case, where the vector $\boldsymbol{\omega} \in S^2$ replaces the index $j = 1, 2$. The absolutely continuous spectrum of H fills $[0, \infty)$ and has a uniform infinite multiplicity, parametrized by the two-dimensional sphere S^2. Solutions $u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})$ are normalized eigenfunctions of the continuous spectrum. In general, the operator H has finitely many negative eigenvalues $\lambda_l < 0$ of finite multiplicities $m_l, l = 1, ..., n$.

In terms of the operators $\mathscr{U}_\pm : \mathscr{H} \to \mathscr{H}$ given by

$$\mathscr{U}_\pm(\psi)(\boldsymbol{k}) = (2\pi)^{-\frac{3}{2}} \int_{\mathbb{R}^3} \psi(\boldsymbol{x})u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})d^3\boldsymbol{x}$$

completeness and orthogonality relations take the form

$$\mathscr{U}_\pm^*\mathscr{U}_\pm = I - P, \quad \mathscr{U}_\pm\mathscr{U}_\pm^* = I,$$

where P is the orthogonal projection on the invariant subspace for the operator H associated with the pure point spectrum. Now let

$$W_\pm = \mathscr{U}_\pm^* \mathscr{U}_0,$$

where $\mathscr{U}_0 = \mathscr{F}^{-1}$ is the inverse Fourier transform. As in Section 2.3, one can prove the following result.

Theorem 4.1. The operators $W_\pm$are wave operators for the Schrodinger operator H. The corresponding scattering operator $S = W_+^* W_-$has the form

$$S = \mathscr{F} \hat{S} \mathscr{F}^{-1}$$

where $\hat{S}$ is the integral operator,

$$(\hat{S}\psi)(k, \boldsymbol{\omega}) = \psi(k, \boldsymbol{\omega}) + \frac{ik}{2\pi} \int_{S^2} f\left(k, \boldsymbol{\omega}, \omega'\right) \psi\left(k, \boldsymbol{\omega}'\right) d\boldsymbol{\omega}'$$

and $f\left(k, \boldsymbol{\omega}, \boldsymbol{\omega}'\right) = f^{(+)}\left(k, \boldsymbol{\omega}, \boldsymbol{\omega}'\right)$.
The function $f\left(k, \boldsymbol{\omega}, \boldsymbol{\omega}'\right)$ is called the scattering amplitude.
Problem 4.1. Prove that if

$$\sup_{\boldsymbol{x} \in \mathbb{R}^3} \int_{\mathbb{R}^3} |V(\boldsymbol{y})| \frac{1}{|\boldsymbol{x} - \boldsymbol{y}|} d^3\boldsymbol{y} < 4\pi$$

then the Lippman-Schwinger integral equations can be solved by Neumann series and for fixed $\boldsymbol{x}$ and $\boldsymbol{\omega}$ solutions $u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k}), \boldsymbol{k} = k\boldsymbol{\omega}$, admit analytic continuation to
the upper half-plane $\operatorname{Im} k > 0$. Show also that in this case the Schrodinger operator H has no eigenvalues.

Problem 4.2 (Born's approximation). Show that $u^{(+)}(\boldsymbol{x}, \boldsymbol{k}) = e^{i\boldsymbol{k}\boldsymbol{x}} + o(1)$ as $k \to \infty$, and deduce from this that

$$f(k, \boldsymbol{n}, \boldsymbol{\omega}) + \frac{1}{4\pi} \int_{\mathbb{R}^3} e^{ik(\boldsymbol{n}-\boldsymbol{\omega})\boldsymbol{x}} V(\boldsymbol{x}) d^3\boldsymbol{x} = o(1) \quad \text{as} \quad k \to \infty$$

uniformly on $\boldsymbol{n}, \boldsymbol{\omega} \in S^2$.
Problem 4.3. Prove unitarity of the operator $\hat{S}$ using Schrodinger equation (4.6), radiation conditions (4.7), and the Green's formula.

Problem 4.4 (The optical theorem). Show that

$$\int_{S^2} |f(k, \boldsymbol{n}, \boldsymbol{\omega})|^2 d\boldsymbol{n} = \frac{4\pi}{k} \operatorname{Im} f(k, \boldsymbol{\omega}, \boldsymbol{\omega}).$$

(Here the left-hand side is the total cross-section in direction $\boldsymbol{\omega}$ at the energy $E = k^2$.)

Problem 4.5. Let $\lambda_l = -\varkappa_l^2 < 0$ be the eigenvalues of H with multiplicities m_l, $l = 1, ..., n$. Prove that for fixed $\boldsymbol{x}$ and $\boldsymbol{\omega}$ solutions $u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})$ admit a meromorphic continuation to the upper half-plane $\operatorname{Im} k > 0$ with poles of orders m_l at $i\varkappa_l$, $l = 1, ..., n$.

Problem 4.6. Prove that the wave operators $W_\pm$exist using the non-stationary approach. (Hint: Show that when $V(\boldsymbol{x})$ satisfies (4.5), Cook's criterion, formulated in Problem 2.7, is applicable.)

4.3. Particle in a central potential.

The eigenvalue problem for the Schrodinger operator

$$H = -\frac{\hbar^2}{2\mu} \Delta + V(\boldsymbol{x})$$

simplifies, when H commutes with the SO(3)-action in $\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{x})$:

$$[H, T(g)] = 0 \quad \text{for all} \quad g \in \mathrm{SO}(3)$$

This reduces to the conditions

$$[H, M_i] = 0, \quad i = 1, 2, 3, \tag{4.9}$$

and is equivalent to the property that the potential V is spherically symmetric, $V(\boldsymbol{x}) = V(r), r = |\boldsymbol{x}|$. In particular

$$[H, M_3] = \left[H, M^2\right] = 0$$

where $M^2 = M_1^2 + M_2^2 + M_3^2$, and operators M_3 and M^2 are commuting quantum integrals of motion for the Hamiltonian H. As follows from results in Section 3.2, one can look for the solutions of the eigenvalue problem

$$H\psi = E\psi$$

satisfying

$$M_3\psi = m\psi \quad \text{and} \quad M^2\psi = \hbar^2 l(l+1)\psi, \quad m = -l, ..., l.$$

Using (3.9), we get

$$H = -\frac{\hbar^2}{2\mu r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\boldsymbol{M}^2}{\mu r^2} + V(r)$$

so that in accordance with the decompositions (3.14) and (3.15), we look for the solutions in the form

$$\psi(\boldsymbol{x}) = R_l(r)Y_{lm}(\boldsymbol{n}), \quad \boldsymbol{x} = r\boldsymbol{n}$$

where Y_{lm} are normalized spherical functions. Separating the variables, one gets the following ordinary differential equation for the function $R_l(r)$:

$$\frac{\hbar^2}{2\mu r^2}\frac{d}{dr}\left(r^2\frac{dR_l}{dr}\right) + \frac{\hbar^2 l(l+1)}{\mu r^2}R_l + V(r)R_l = ER_l.$$

Introducing

$$f_l(r) = rR_l(r)$$

we obtain the so-called radial Schrodinger equation

$$-\frac{\hbar^2}{2\mu}\frac{d^2 f_l}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2}f_l + V(r)f_l = Ef_l \tag{4.10}$$

Since for the continuous potential $V(\boldsymbol{x})$ the solution $\psi(\boldsymbol{x})$ is also continuous, equation (4.10) should be supplemented by the boundary condition $f_l(0) = 0$.

The radial Schrodinger equation looks similar to the Schrodinger equation for a one-dimensional particle, if one introduces the so-called effective potential

$$V_{\text{eff}}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2}$$

where the second term is called the centrifugal energy. However, since f_l is defined only for $r > 0$, equation (4.10) is equivalent to equation (2.1) with the potential satisfying $V(x) = \infty$ for $x < 0$, which describes the infinite potential barrier at $x = 0$.

Since the radial Schrodinger operators

$$H_l = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2}$$

are obtained from the three-dimensional Schrodinger operator

$$H = -\frac{\hbar^2}{2\mu}\Delta + V(r)$$

by separation of variables, the operators H_l with boundary condition $f_l(0) = 0$ are self-adjoint in $L^2(0,\infty)$ whenever H is a self-adjoint operator in $L^2(\mathbb{R}^3)$.

In particular, it follows from Theorem 1.9 in Section 1.2 that when the bounded potential V satisfies

$$V(r) = O\left(r^{-1-\varepsilon}\right) \quad \text{as} \quad r \to \infty$$

for some $\varepsilon > 0$, then H_l are self-adjoint operators with simple absolutely continuous spectrum filling $[0,\infty)$, and negative eigenvalues with possible accumulation point at 0 . If

$$V(r) = O\left(r^{-2-\varepsilon}\right) \quad \text{as} \quad r \to \infty,$$

then the operators H_l have only finitely many negative eigenvalues, and for l large enough have no eigenvalues at all. The same conclusion holds if

$$\int_0^\infty r|V(r)|dr < \infty \tag{4.11}$$

Such potentials $V(r)$ are called short-range potentials. Decaying at infinity potentials which do not satisfy (4.11) are called long-range potentials.

For a short-range potential $V(r)$ the differential equation (4.10) for $E \neq 0$ has two linearly independent solutions $f_l^{\pm}(r)$ satisfying the following asymptotics as $r \to \infty$:

$$f_l^{\pm}(r) = e^{\pm \varkappa r}(1 + o(1)), \tag{4.12}$$

where $\varkappa = \sqrt{-2\mu E}$ is pure imaginary, $\operatorname{Im} \varkappa > 0$ for $E > 0$, and $\varkappa > 0$ for $E < 0$. When $r \to 0$, the most singular term in the radial Schrodinger equation is given by the centrifugal energy. Since the elementary differential equation

$$f'' = \frac{l(l+1)}{r^2} f$$

has two linearly independent solutions r^{-l} and r^{l+1}, the solution $f_l(r)$ satisfying the boundary condition $f_l(0) = 0$ has the asymptotics

$$f_l(r) = Cr^{l+1} + o(1) \quad \text{as} \quad r \to 0, \tag{4.13}$$

and is uniquely determined (up to a constant). Since

$$f_l(r) = C_1 f_l^+(r) + C_2 f_l^-(r),$$

for some constants C_1 and C_2 depending on E, the differential equation (4.10) has no square-integrable solutions for $E > 0$. The corresponding solution $f_l(r)$ is bounded on $[0,\infty)$, and is an eigenfunction of the continuous spectrum. This agrees with the description in Section 1.6 of

Chapter 1, since for $E > 0$ the classical particle in the central potential $V_{\text{eff}}(r)$ goes to infinity with finite velocity. For $E < 0$ the equation $C_1(E) = 0$ determines the eigenvalues of H_l, which are simple. This also agrees with the classical picture, since classical motion is finite for $E < 0$. For a short range potential the equation $C_1(E) = 0$ has only finitely many solutions. When $V_{\text{eff}}(r) > 0$ for $r > 0$ - the case of repulsive potential - the operator H_l has no eigenvalues.

Remark. When $V(r) = 0$, the radial Schrodinger operator H_l has only simple absolutely continuous spectrum filling $[0, \infty)$. The substitution

$$f_l(r) = \sqrt{\xi} J(\xi), \quad \xi = \frac{kr}{\hbar} \quad \text{and} \quad k = |\varkappa| = \sqrt{2\mu E} > 0$$

reduces differential equation (4.10) to the Bessel equation

$$\xi^2 \frac{d^2 J}{d\xi^2} + \xi \frac{dJ}{d\xi} + \left(\xi^2 - \nu^2\right) J = 0$$

of the half-integer order $\nu = l + \frac{1}{2}$. The corresponding solution regular at 0 - the Bessel function of the first kind $J_{l+\frac{1}{2}}(\xi)$ - is given explicitly by

$$J_{l+\frac{1}{2}}(\xi) = (-1)^l \sqrt{\frac{2}{\pi\xi}} \xi^{l+1} \left(\frac{1}{\xi}\frac{d}{d\xi}\right)^l \frac{\sin\xi}{\xi}$$

and

$$J_{l+\frac{1}{2}}(\xi) = \sqrt{\frac{2}{\pi\xi}} \sin\left(\xi - \frac{l\pi}{2}\right) \quad \text{as} \quad \xi \to \infty \tag{4.14}$$

It can be shown that

$$f_{El}(r) = \sqrt{\frac{kr}{\hbar}} J_{l+\frac{1}{2}}\left(\frac{kr}{\hbar}\right)$$

satisfy the normalization condition (2.14) in Section 2.2 of Chapter 2:

$$\lim_{\Delta\to 0} \frac{1}{\Delta} \int_0^\infty \left(\int_k^{k+\Delta} f_{El}(r) d\sigma(E) \right)^2 dr = 1 \tag{4.15}$$

where $k = \sqrt{2\mu E}$ and $d\sigma(E) = \sqrt{\frac{\mu}{2E}} dE = dk$. The corresponding eigenfunction expansion theorem is the special case of the classical Fourier-Bessel transform for integer l, which generalizes the Fourier sine transform: for every $f \in L^2(0, \infty)$,

$$f(r) = \int_0^\infty c_l(E) f_{El}(r) d\sigma(E), \quad c_l(E) = \int_0^\infty f(r) f_{El}(r) dr$$

In general, for every $l = 0, 1, ...$, denote by $f_{El}(r)$ the solution of the radial Schrodinger equation (4.10) with the following asymptotics:

$$f_{El}(r) = \sqrt{\frac{2}{\pi\hbar}} \sin\left(\frac{kr}{\hbar} - \frac{l\pi}{2} + \delta_l\right) + o(1) \quad \text{as} \quad r \to \infty \tag{4.16}$$

The function $\delta_l(k), k = \sqrt{2\mu E}$, is called the phase shift. It follows from (4.14) that for the free case $\delta_l(k) = 0$. The eigenfunctions of the continuous spectrum $f_{El}(r)$ satisfy the same normalization condition (4.15) as the
eigenfunctions for the free case. The function $S_l(k) = e^{2i\delta_l(k)}$ plays the role of the scattering matrix for the radial Schrodinger operator H_l. It admits a meromorphic continuation to the upper half-plane $\operatorname{Im} k > 0$ with simple poles $k = i\varkappa_{kl} = i\sqrt{-2\mu E_{kl}}$, where E_{kl} are the eigenvalues of H_l.

Let $E_{0l} < E_{2l} < \cdots < E_{N_l-1l} < 0$ be the eigenvalues of H_l, and let $f_{jl}(r), j = 0, ..., N_l - 1$, be the corresponding normalized eigenfunctions. By the oscillation theorem, the eigenfunctions $f_{jl}(r)$ have j simple zeros in $(0, \infty)$. The functions

$$\psi_{jlm}(\boldsymbol{x}) = \frac{f_{jl}(r)}{r} Y_{lm}(\boldsymbol{n}), \quad m = -l, ..., l$$

are normalized eigenfunctions of the Schrodinger operator H with eigenvalues E_{jl}, and the functions

$$\psi_{Elm}(\boldsymbol{x}) = \frac{f_{El}(r)}{r} Y_{lm}(\boldsymbol{n}), \quad m = -l, ..., l,$$

are normalized eigenfunctions of the continuous spectrum. The corresponding eigenfunction expansion theorem for the Schrodinger operator H with spherically symmetric potential states that for every $\psi \in L^2(\mathbb{R}^3, d^3\boldsymbol{x})$,

$$\psi(\boldsymbol{x}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \int_0^{\infty} c_{lm}(E) \psi_{Elm}(\boldsymbol{x}) d\sigma(E) + \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{j=0}^{N_l-1} c_{jlm} \psi_{jlm}(\boldsymbol{x})$$

where

$$c_{lm}(E) = \int_{\mathbb{R}^3} \psi(\boldsymbol{x}) \overline{\psi_{Elm}(\boldsymbol{x})} d^3\boldsymbol{x}, \quad c_{jlm} = \int_{\mathbb{R}^3} \psi(\boldsymbol{x}) \overline{\psi_{jlm}(\boldsymbol{x})} d^3\boldsymbol{x}.$$

Remark. In physics, it is traditional to call the parameter j in the eigenfunction $\psi_{jlm}(\boldsymbol{x})$ the radial quantum number and denote it by n_r. The parameter l is called the azimuthal quantum number, and the parameter m - the magnetic quantum number. This terminology originated from the old quantum theory, where to each value E_{kl} there corresponds a classical orbit. The parameter $n = n_r + l + 1$ is called the principal quantum number, so that $n_r = n - l - 1$ is always the number of zeros of the corresponding radial eigenfunction $f_{jl}(r)$.

Remark. In general, the eigenvalues E_{jl} of a Schrodinger operator H with spherically symmetric potential have multiplicity $2l+1$. For special potentials, due to the extra symmetry of a problem, there may be "accidental degeneracy" with respect to the azimuthal quantum number l. This is the case for the Schrodinger operator of the hydrogen atom, considered in the next section.

Problem 4.7. Prove all results stated in this section. (Hint: See the list of references to this chapter.)

Problem 4.8. Find the energy levels of a particle with angular momentum $l = 0$ in the centrally symmetric potential well $V(r) = -V_0 < 0$ when $0 < r < a$ and $V(r) = 0$ when $r > a$.

Problem 4.9. Find the spectrum of the Schrodinger operator with the potential $V(r) = ar^{-2} + br^2, a, b > 0$.

Problem 4.10. Prove that the scattering wave $u(\boldsymbol{x}, \boldsymbol{k}) = u^{(+)}(\boldsymbol{x}, \boldsymbol{k})$ in the central potential is given by

$$u(\boldsymbol{x}, \boldsymbol{k}) = \frac{1}{kr} \sqrt{\frac{\pi}{2}} \sum_{l=0}^{\infty} (2l+1) i^l e^{i\delta_l(k)} f_{El}(r) P_l(\cos\vartheta),$$

where $\boldsymbol{x} \cdot \boldsymbol{k} = kr\cos\vartheta$ and, as in Section 4.2, $\hbar = 1$ and $\mu = \frac{1}{2}$.

Problem 4.11. Using the result of the previous problem, show that

$$f(k, \boldsymbol{n}, \boldsymbol{\omega}) = f(k, \cos\vartheta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) \left(S_l(k) - 1\right) P_l(\cos\vartheta)$$

- the partial wave decomposition of the scattering amplitude - and get the following formula for the total cross-section

$$\sigma_{\text{tot}}(k) = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l(k).$$

3.6.11 5. Hydrogen atom and SO(4)

Theory

The hydrogen atom is described by the long-range potential

$$V(\boldsymbol{r}) = -\frac{\alpha}{r}$$

- the Coulomb potential, where $\alpha > 0$[3]. The corresponding eigenvalue problem for the Schrodinger operator with Coulomb potential is called the Coulomb problem. Here we present its exact solution using the so-called Coulomb units $\hbar = 1, \mu = 1$, and $\alpha = 1$[4].

5.1. Discrete spectrum.

To determine the discrete spectrum, it is convenient to put $2E = -\varkappa^2 < 0$, so that the eigenvalue equation (4.10) becomes

$$f_l'' + \left(\frac{2}{r} - \frac{l(l+1)}{r^2} - \varkappa^2\right) f_l = 0. \tag{5.1}$$

Asymptotics (4.12)-(4.13) for the short-range potentials suggest that for the long-range Coulomb potential one can look for a square-integrable solution in the following form:

$$f_l(r) = r^{l+1}e^{-\varkappa r}\Lambda(r)$$

Substituting it into (5.1), we get the equation

$$\Lambda_l'' + \left(\frac{2(l+1)}{r} - 2\varkappa\right)\Lambda_l' + \left(\frac{2}{r} - \frac{2\varkappa(l+1)}{r}\right)\Lambda_l = 0, \tag{5.2}$$

which can be solved by the power series

$$\Lambda_l(r) = \sum_{k=0}^{\infty} a_k r^k \tag{5.3}$$

Substituting these power series into (5.2) yields the following recurrence relation for the coefficients a_k:

$$a_{k+1} = \frac{2\varkappa(k+l+1)-2}{(k+1)(k+2l+2)}a_k, \quad k = 1, 2, ...,$$

where $a_0 \neq 0$. The power series (5.3) converges for all $r > 0$ by the ratio test. When $\varkappa > 0$ is such that $a_k \neq 0$ for all k, we have

[3] For the hydrogen atom $\alpha = e^2$, where e is the electron charge. The case $\alpha = Ze^2$, where $Z = 2, 3, ...$, corresponds to the hydrogen ions.
[4] When $\alpha = e^2$, Coulomb units coincide with atomic units.

$$\lim_{k\to\infty}\frac{(k+1)a_{k+1}}{a_k}=2\varkappa.$$

Thus for every $\varepsilon>0$ there is N such that for $k>N$ all a_k are of the same sign, say $a_k>0$, and

$$\frac{a_{k+1}}{a_k}\geq\frac{2\varkappa-\varepsilon}{k+1}.$$

Then for $k>N$ we get

$$a_k\geq C\frac{(2\varkappa-\varepsilon)^k}{k!}$$

with some constant $C>0$ (depending on ε), and since for fixed N the sum of the first N terms in (5.3) grows like r^N as $r\to\infty$, for r large enough we obtain [5]

$$\Lambda_l(r)\geq Ce^{(2\varkappa-\varepsilon)r}-C_1r^N>C_2e^{(2\varkappa-\varepsilon)r}.$$

This proves that for such values of $\varkappa$ the function $f_l(r)$ is not squareintegrable on $(0,\infty)$. However, for the special values

$$\varkappa=\varkappa_{kl}=\frac{1}{k+l+1}$$

the power series (5.3) terminates: $\Lambda_l(r)$ becomes a polynomial $\Lambda_{kl}(r)$ of order k and $f_{kl}(r)=r^{l+1}e^{-\varkappa_{kl}r}\Lambda_{kl}(r)\in L^2(0,\infty)$. Setting $n=k+l+1$, we get an explicit formula for the eigenvalues

$$E_n=-\frac{1}{2n^2},\quad n=1,2,...$$

For fixed n the integer l varies from 0 to $n-1$, and for each l there are $2l+1$ orthogonal eigenfunctions $\frac{f_{kl}(r)}{r}Y_{lm}(n)$ with the eigenvalue E_n. Thus the overall multiplicity of the eigenvalue E_n is

$$\sum_{l=0}^{n-1}(2l+1)=n^2.$$

The eigenfunctions $f_{kl}(r)$ of the radial Schrodinger equation (5.1) corresponding to the eigenvalue E_n can be expressed in terms of classical Laguerre polynomials. Namely, for $\varkappa=\frac{1}{n}$ the substitution $x=\frac{2r}{n}$ reduces the differential equation (5.2) to

$$xQ''+(p+1-x)Q'+kQ=0$$

where $p=2l+1$ and $Q(x)=\Lambda_l(r)$. This is the differential equation satisfied by the associated Laguerre polynomials $Q_k^p(x)$, defined by [6]

$$Q_k^p(x)=e^xx^{-p}\frac{d^k}{dx^k}\left(e^{-x}x^{k+p}\right)$$

which are polynomials of order k with leading coefficient $(-1)^k$, having k zeros in $(0,\infty)$. For every p the associated Laguerre polynomials $\{Q_k^p(x)\}_{k=0}^\infty$ are orthogonal polynomials on $(0,\infty)$ with respect to the measure $e^{-x}x^pdx$, and have the property

$$\int_0^\infty e^{-x}x^{p+1}Q_k^p(x)^2dx=k!(k+p)!(2k+p+1)$$

[05] It can be shown that $\Lambda_l(r)=Ce^{2\varkappa r}(1+o(1))$ as $r\to\infty$.

The orthonormal eigenfunctions of the Schrodinger operator H for the hydrogen atom corresponding to the eigenvalue E_n have the form

$$\psi_{klm}(\boldsymbol{q}) = \frac{2}{n^2}\frac{1}{\sqrt{k!(n+l)!}}\left(\frac{2r}{n}\right)^l e^{-\frac{r}{n}} Q_k^{2l+1}\left(\frac{2r}{n}\right) Y_{lm}(\boldsymbol{n}), \tag{5.4}$$

where $n = k + l + 1, l = 0, ..., n-1$, and $m = -l, ..., l$.
Remark. Returning to the physical units $\alpha = e^2$, where e is the electron charge, we get for the energy levels of the hydrogen atom

$$E_n = -\frac{\mu e^4}{2n^2\hbar^2}$$

where μ is the reduced mass of the electron and the nucleus. In particular, the ground state energy is $E_1 = -13.6\text{eV}$; its absolute value is the ionization energy - the energy required to remove the electron from the hydrogen atom. Using Bohr's formula for the frequencies of the spectral lines

$$\hbar\omega_{mn} = E_n - E_m,$$

we get for the hydrogen atom

$$\omega_{mn} = \frac{\mu e^4}{2\hbar^3}\left(\frac{1}{n^2} - \frac{1}{m^2}\right), \quad m < n$$

When $n = 1$ and $m = 2, 3, ...$, we get classical Lyman series, $n = 2$ and $m = 3, 4, ...$ give Balmer series, and $n = 3$ and $m = 4, 5, ...$ give Paschen series. These series of spectral lines were discovered experimentally long before the formulation of quantum mechanics.

Remark. The energy levels of the hydrogen atom can also be determined from Bohr-Wilson-Sommerfeld quantization rules. Namely, in spherical coordinates (r, ϑ, φ) in $\mathbb{R}^3$ the Lagrangian of Kepler's problem takes the form (see Section 1.6 in Chapter 1)

$$L = \frac{1}{2}\mu\left(\dot{r}^2 + r^2\dot{\vartheta}^2 + r^2\sin^2\vartheta\dot{\varphi}^2\right) + \frac{\alpha}{r}$$

and the corresponding generalized momenta are

$$p_r = \mu\dot{r}, \quad p_\vartheta = \mu r^2\dot{\vartheta}, \quad p_\varphi = \mu r^2\sin^2\vartheta\dot{\varphi}.$$

The BWS quantization conditions

$$\oint p_r dr = 2\pi\hbar\left(k + \frac{1}{2}\right) \tag{5.5}$$

$$\oint p_\vartheta d\vartheta = 2\pi\left(l - m + \frac{1}{2}\right) \tag{5.6}$$

$$\oint p_\varphi d\varphi = 2\pi\hbar m \tag{5.7}$$

where integration goes over the closed orbit of the Kepler problem with the energy $E < 0$, exactly determine the energy levels $E_n, n = k + l + 1$.

Indeed, we have $p_\varphi = M_{c3}$, where $M_c = (M_{c1}, M_{c2}, M_{c3})$ is the classical angular momentum. It is constant along the orbit, so that (5.7) determines the eigenvalues of operator M_3 (see Section 3.2). To evaluate $\oint p_\vartheta d\vartheta$, we use polar coordinates (r, χ) in the orbit plane P (see

[06] Polynomials $L_n^m(x) = (-1)^m\frac{n!}{(n-m)!}Q_{n-m}^m(x)$ are also being used.

Section 1.6 in Chapter 1). Since $\dot{\chi}^2 = \dot{\vartheta}^2 + \sin^2\vartheta\dot{\varphi}^2$, along the orbit we get $p_\chi d\chi = p_\vartheta d\vartheta + p_\varphi d\varphi$, where $p_\chi = \mu r^2\dot{\chi} = |\boldsymbol{M}_{\rm c}|$. Condition (5.6) now follows from

$$\oint p_\chi d\chi = 2\pi\,|M_{\rm c}| = 2\pi\hbar\left(l+\frac{1}{2}\right) \tag{5.8}$$

which is the quantization rule for the square of total angular momentum [7]. Finally, to evaluate $\oint p_r dr$, we use equations (1.7) and (1.11) in Section 1.6

of Chapter 1 and get

$$p_r dr = \mu\dot{r}dr = \mu\frac{dr}{d\chi}\dot{\chi}dr = \frac{|M_{\rm c}|}{r^2}\left(\frac{dr}{d\chi}\right)^2 d\chi = p_\chi\frac{e^2\sin^2\chi}{(1+e\cos\chi)^2}d\chi$$

where $0 < e < 1$ is the eccentricity of the orbit. We have

$$\oint p_r dr = p_\chi\int_0^{2\pi}\frac{e^2\sin^2\chi}{(1+e\cos\chi)^2}d\chi = 2\pi p_\chi\left(\frac{1}{\sqrt{1-e^2}}-1\right)$$

as can be shown by using the substitution $z = e^{i\chi}$ and the Cauchy residue theorem [8]. It follows from equation (1.12) in Section 1.6 of Chapter 1 that

$$\sqrt{1-e^2} = \frac{|\boldsymbol{M}_{\rm c}|\,\sqrt{2|E|}}{\alpha\sqrt{\mu}}$$

and we obtain from (5.5) and (5.8),

$$|E| = -E_n = \frac{\mu\alpha^2}{2n^2\hbar^2}, \quad n = k+l+1$$

5.2. Continuous spectrum.

Set $2E = k^2$, where $k > 0$, and consider the equation

$$f_l'' + \left(\frac{2}{r} - \frac{l(l+1)}{r^2} + k^2\right) f_l = 0 \tag{5.9}$$

Substitution

$$f_l(r) = r^{l+1}e^{-ikr}F_l(r)$$

reduces (5.9) to

$$F_l'' + \left(\frac{2(l+1)}{r} - 2ik\right)F_l' + \left(\frac{2}{r} - \frac{2ik(l+1)}{r}\right)F_l = 0. \tag{5.10}$$

The solution of equation (5.10) satisfying $F_l(0) = 1$ can be explicitly written as

$$F_l(r) = F(l+1+i\lambda, 2l+2, 2ikr), \quad \lambda = \frac{1}{k}$$

where $F(\alpha,\gamma,z)$ is a confluent hypergeometric function, defined by the absolutely convergent series

[07] It gives the quantized values $\hbar^2\left(l+\frac{1}{2}\right)^2$, which for large l agree well with the eigenvalues $\hbar^2 l(l+1)$ of the operator $\boldsymbol{M}^2$.

$$F(\alpha,\gamma,z)=\sum_{n=0}^{\infty}\frac{\Gamma(\alpha+n)\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma+n)}\frac{z^n}{n!}$$

for all α and $\gamma\neq 0,-1,-2,\ldots$ The confluent hypergeometric function is an entire function of the variable z and satisfies the differential equation

$$zF''+(\gamma-z)F'-\alpha F=0$$

For $\alpha=-k$ and $\gamma=p+1$, where $k,p=0,1,2,\ldots$, the confluent hypergeometric function reduces to associated Laguerre polynomials

$$Q_k^p(x)=\frac{(k+p)!}{p!}F(-k,p+1,x)$$

considered in the previous section. For $\operatorname{Re}\gamma>\operatorname{Re}\alpha>0$ the function $F(\alpha,\gamma,z)$ admits the integral representation

$$F(\alpha,\gamma,z)=\frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma-\alpha)}\int_0^1 t^{\alpha-1}(1-t)^{\gamma-\alpha-1}e^{zt}dt \tag{5.11}$$

obtained by the Laplace method. The confluent hypergeometric function satisfies the functional equation

$$F(\alpha,\gamma,z)=e^zF(\gamma-\alpha,\gamma,-z) \tag{5.12}$$

and has the following asymptotics as $z\to\infty$:

$$\begin{aligned}F(\alpha,\gamma,z)=\frac{\Gamma(\gamma)}{\Gamma(\gamma-\alpha)}(-z)^{-\alpha}\left(1+O\left(z^{-1}\right)\right)\\ +\frac{\Gamma(\gamma)}{\Gamma(\alpha)}e^zz^{\alpha-\gamma}\left(1+O\left(z^{-1}\right)\right)\end{aligned} \tag{5.13}$$

It follows from (5.12) that $f_l(r)=r^{l+1}e^{-ikr}F(l+1+i\lambda,2l+2,2ikr)$ is real-valued and it follows from (5.13) that the function

$$f_{El}(r)=\frac{(2k)^{l+1}}{\sqrt{2\pi}(2l+1)!}e^{\frac{\pi}{2k}}|\Gamma(l+1-i\lambda)|f_l(r) \tag{5.14}$$

has the following asymptotics as $r\to\infty$:

$$f_{El}(r)=\sqrt{\frac{2}{\pi}}\sin\left(kr+\lambda\log 2kr-\frac{l\pi}{2}+\delta_l\right) \tag{5.15}$$

where

$$\delta_l(k)=\arg\Gamma(l+1-i\lambda),\quad \lambda=\frac{1}{k}=\frac{1}{\sqrt{2E}} \tag{5.16}$$

is the phase shift. The partial S-matrix for the Coulomb problem is

$$S_l(k)=e^{2i\delta_l(k)}=\frac{\Gamma(l+1-i\lambda)}{\Gamma(l+1+i\lambda)}$$

[08] This integral was evaluated by Sommerfeld in 1916.

It admits meromorphic continuation to the upper half-plane $\operatorname{Im} k > 0$ and has simple poles at $k = i\varkappa_{jl}$, which correspond to the eigenvalues E_{kl} of the radial Schrodinger operator H_l. The radial eigenfunctions of the continuous spectrum (5.14) satisfy normalization condition (4.15).
Remark. It is instructive to compare asymptotics (5.15) for the Coulomb potential, which is long-range, with the corresponding formula (4.16) for the general short-range potential. The long range nature of the Coulomb interaction manifests itself by the extra logarithmic term $\lambda \log 2kr$ in (5.15).

The eigenfunction expansion theorem for the Schrodinger operator H of the hydrogen atom has the same form as in Section 4.3: the eigenfunctions $\psi_{klm}(\boldsymbol{x})$ are given by (5.4) where $k = 0, 1, ..., N_l = \infty$, and the eigenfunctions of the continuous spectrum are given by

$$\psi_{Elm}(\boldsymbol{x}) = \frac{f_{El}(r)}{r} Y_{lm}(\boldsymbol{n}), \quad l = 0, 1, ..., \quad m = -l, ..., l.$$

5.3. Hidden SO(4) symmetry.

As we have seen in Section 1.6 of Chapter 1, classical system with the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{x}) = \frac{\boldsymbol{p}^2}{2m} - \frac{\alpha}{r},$$

in addition to the angular momentum $\boldsymbol{M}_{\mathbf{c}}$, has three extra integrals of motion given by the Laplace-Runge-Lenz vector

$$\boldsymbol{W}_{\mathrm{c}} = \frac{\boldsymbol{p}}{m} \times \boldsymbol{M}_{\mathrm{c}} - \frac{\alpha \boldsymbol{x}}{r}.$$

According to Example 2.2 in Section 2.6 of Chapter 1, the integrals $\boldsymbol{M}_{\mathrm{c}}$ and $\boldsymbol{W}_{\mathrm{c}}$ for the Kepler problem have the Poisson brackets

$$\{M_{\mathrm{c}j}, M_{\mathrm{c}k}\} = -\varepsilon_{jkl} M_{\mathrm{c}l}, \quad \{W_{\mathrm{c}j}, M_{\mathrm{c}k}\} = -\varepsilon_{jkl} W_{\mathrm{c}l}$$
$$\{W_{\mathrm{c}j}, W_{\mathrm{c}k}\} = 2H_{\mathrm{c}} \varepsilon_{jkl} M_{\mathrm{c}l}$$

where $j, k, l = 1, 2, 3$ and $\varepsilon_{123} = 1$.
The quantum Kepler problem is the Coulomb problem. In the coordinate representation $\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{x})$, its Hamiltonian is

$$H = \frac{\boldsymbol{P}^2}{2} - \frac{\alpha}{r}$$

where $r = |\boldsymbol{x}|$ and we put $m = 1$. The quantum Laplace-Runge-Lenz vector - the Laplace-Runge-Lenz operator $\boldsymbol{W}$ - is defined by

$$\boldsymbol{W} = \frac{1}{2}(\boldsymbol{P} \times \boldsymbol{M} - \boldsymbol{M} \times \boldsymbol{P}) - \frac{\alpha \boldsymbol{Q}}{r}$$

or in components

$$W_j = \frac{1}{2} \varepsilon_{jkl} (P_k M_l + M_l P_k) - \frac{\alpha Q_j}{r}, \quad j = 1, 2, 3$$

Here Q_i are multiplication by x_i operators, and it is always understood that there is a summation over repeated indices $1, 2, 3$. Using commutation relations (3.5), we also have

$$\boldsymbol{W} = \boldsymbol{P} \times \boldsymbol{M} - \frac{\alpha \boldsymbol{Q}}{r} - i\hbar \boldsymbol{P} = -\boldsymbol{M} \times \boldsymbol{P} - \frac{\alpha \boldsymbol{Q}}{r} + i\hbar \boldsymbol{P} \tag{5.17}$$

where the term $i\hbar \boldsymbol{P}$ plays the role of a "quantum correction". The following result reveals the hidden symmetry of the Coulomb problem.

Proposition 5.1. The Schrodinger operator H of the hydrogen atom has quantum integrals of motion $\boldsymbol{M}$ and $\boldsymbol{W}$,

$$[H, M_i] = [H, W_i] = 0, \quad i = 1, 2, 3,$$

satisfying $\boldsymbol{W} \cdot \boldsymbol{M} = \boldsymbol{M} \cdot \boldsymbol{W} = 0$ and

$$\boldsymbol{W}^2 = \alpha^2 + 2H\boldsymbol{M}^2 + 2\hbar^2 H. \tag{5.18}$$

Moreover, self-adjoint operators $\boldsymbol{M}$ and $\boldsymbol{W}$ have the following commutation relations:

$$[M_j, M_k] = i\hbar\varepsilon_{jkl}M_l, \quad [W_j, M_k] = i\hbar\varepsilon_{jkl}W_l, \quad [W_j, W_k] = -2i\hbar\varepsilon_{jkl}M_l H.$$

Proof. We know that $[H, M_j] = 0$. To prove that W_j are quantum integrals of motion, we first compute $\left[\boldsymbol{P}^2, \frac{Q_j}{r}\right]$. It follows from Heisenberg's commutation relations that

$$\left[P_j, \frac{1}{r}\right] = i\hbar\frac{Q_j}{r^3}, \tag{5.19}$$

so that using Leibniz rule and relations $r^2 = x_1^2 + x_2^3 + x_3^2$, $[M_l, r] = 0$, and $Q_j P_k - Q_k P_j = \varepsilon_{jkl}M_l$, we obtain

$$\left[\boldsymbol{P}^2, \frac{Q_j}{r}\right] = 2i\hbar\frac{Q_j}{r^3} + 2i\hbar\varepsilon_{jkl}\frac{Q_k}{r^3}M_l.$$

Now using the first equation in (5.17) and (5.19), we get

$$\begin{aligned}[H, W_j] &= \left[\frac{\boldsymbol{P}^2}{2} - \frac{\alpha}{r}, \varepsilon_{jkl}P_k M_l - \frac{\alpha Q_j}{r} - i\hbar P_j\right] \\ &= -i\alpha\hbar\frac{Q_j}{r^3} - i\alpha\hbar\varepsilon_{jkl}\frac{Q_k}{r^3}M_l + i\alpha\hbar\varepsilon_{jkl}\frac{Q_k}{r^3}M_l + i\alpha\hbar\frac{Q_j}{q^3} = 0.\end{aligned}$$

It is easy to prove the relation $\boldsymbol{W} \cdot \boldsymbol{M} = W_1M_1 + W_2M_2 + W_3M_3 = 0$. Indeed, it follows from the definition of $\boldsymbol{M}$ and commutativity of P_k and Q_l for $k \neq l$ that

$$\boldsymbol{M} \cdot \boldsymbol{P} = \boldsymbol{P} \cdot \boldsymbol{M} = \boldsymbol{M} \cdot \boldsymbol{Q} = \boldsymbol{Q} \cdot \boldsymbol{M} = 0,$$

and using the first equation in (5.17) and commutation relations for the components of the angular momentum, we immediately get $\boldsymbol{W} \cdot \boldsymbol{M} = 0$. To prove that $\boldsymbol{M} \cdot \boldsymbol{W} = 0$, one should use the second equation in (5.17).

Verification of (5.18) is more involved. We have

$$\begin{aligned}W^2 = W_j W_j &= \left(\varepsilon_{jkl}M_l P_k - \frac{\alpha Q_j}{r} + i\hbar P_j\right)\left(\varepsilon_{jmn}P_m M_n - \frac{\alpha Q_j}{r} - i\hbar P_j\right) \\ &= \varepsilon_{jkl}\left(\varepsilon_{jmn}M_l P_k P_m M_n - \alpha M_l P_k \frac{Q_j}{r} - i\hbar M_l P_k P_j\right) - \alpha\varepsilon_{jmn}\frac{Q_j}{q}P_m M_n \\ &+ \alpha^2\frac{Q_j Q_j}{r^2} + i\alpha\hbar\frac{Q_j}{r}P_j + i\hbar\varepsilon_{jmn}P_j P_m M_n - i\alpha\hbar P_j\frac{Q_j}{r} + \hbar^2 P_j P_j \\ &= \alpha^2 I + \hbar^2 P^2 + \varepsilon_{jkl}\varepsilon_{jmn}M_l P_k P_m M_n - \alpha\varepsilon_{jkl}\left(M_l P_k \frac{Q_j}{q} + \frac{Q_j}{r}P_k M_l\right) \\ &- i\alpha\hbar\left[P_j, \frac{Q_j}{r}\right]\end{aligned}$$

Since operators M_j and P_j commute, the identity $(\boldsymbol{a} \times \boldsymbol{b})^2 = \boldsymbol{a}^2\boldsymbol{b}^2 - (\boldsymbol{a} \cdot \boldsymbol{b})^2$ is still applicable and we get

$\varepsilon_{jkl}\varepsilon_{jmn}M_lP_kP_mM_n = -(\boldsymbol{M}\times\boldsymbol{P})\cdot(\boldsymbol{P}\times\boldsymbol{M}) = \boldsymbol{M}^2\boldsymbol{P}^2 - (\boldsymbol{M}\cdot\boldsymbol{P})^2 = \boldsymbol{M}^2\boldsymbol{P}^2$.
Using (5.19) we easily obtain (summation over repeated indices)

$$\left[P_j, \frac{Q_j}{r}\right] = i\hbar\left(-\frac{3}{r} + \frac{r^2}{r^3}\right) = -\frac{2i\hbar}{r}.$$

Since $[\boldsymbol{M}^2, r] = 0$ it follows from $\boldsymbol{M} = \boldsymbol{Q}\times\boldsymbol{P}$ that

$$\varepsilon_{jkl}\left(M_lP_k\frac{Q_j}{r} + \frac{Q_j}{r}P_kM_l\right) = M^2\frac{1}{r} + \frac{1}{r}M^2 = \frac{2M^2}{r}.$$

Putting everything together, we get (5.18).
It is also not difficult to establish commutation relations between M_j and W_k. Using (3.5) and properties of ε_{jkl}, we get

$$\begin{aligned}[M_j, W_k] &= \left[M_j, \varepsilon_{kmn}P_mM_n - \frac{\alpha Q_k}{r} - i\hbar P_k\right]\\ &= i\hbar\left(\varepsilon_{jmp}\varepsilon_{kmn}P_pM_n + \varepsilon_{jnp}\varepsilon_{kmn}P_mM_p\right) - i\hbar\varepsilon_{jkl}\left(\frac{\alpha Q_l}{r} + i\hbar P_l\right)\\ &= i\hbar\left(P_jM_k - M_kP_j\right) - i\hbar\varepsilon_{jkl}\left(\frac{\alpha r_l}{r} + i\hbar P_l\right) = i\hbar\varepsilon_{jkl}W_l\end{aligned}$$

Finally, to establish commutation relations between components of $\boldsymbol{W}$, we use the representations

$$\boldsymbol{W} = \boldsymbol{Q}\boldsymbol{P}^2 - \boldsymbol{P}(\boldsymbol{Q}\cdot\boldsymbol{P}) - \frac{\alpha\boldsymbol{Q}}{r} = \boldsymbol{P}^2\boldsymbol{Q} - (\boldsymbol{P}\cdot\boldsymbol{Q})\boldsymbol{P} - \frac{\alpha\boldsymbol{Q}}{r} \tag{5.20}$$

The first formula in (5.20) follows from the first formula in (5.17) by using

$$\begin{aligned}\varepsilon_{jkl}P_kM_l = \varepsilon_{jkl}\varepsilon_{lmn}P_kQ_mP_l &= \varepsilon_{jkl}\left(\varepsilon_{ljk}P_kQ_jP_k + \varepsilon_{lkj}P_kQ_kP_j\right)\\ &= P_k\left(P_kQ_j - P_jQ_k\right) = Q_j\boldsymbol{P}^2 - P_j(\boldsymbol{P}\cdot\boldsymbol{Q}) - 2i\hbar P_j\end{aligned}$$

and relation $\boldsymbol{P}\cdot\boldsymbol{Q} = \boldsymbol{Q}\cdot\boldsymbol{P} - 3i\hbar I$. The second formula in (5.20) follows from the first by using Heisenberg's commutation relations. Now we have

$$\begin{aligned}\varepsilon_{jkl}\left[W_k, W_l\right] &= 2\varepsilon_{jmn}W_mW_n\\ = 2\varepsilon_{jmn}&\left(\boldsymbol{P}^2Q_m - (\boldsymbol{P}\cdot\boldsymbol{Q})P_m - \frac{\alpha Q_m}{r}\right)\left(Q_n\boldsymbol{P}^2 - P_n(\boldsymbol{Q}\cdot\boldsymbol{P}) - \frac{\alpha Q_n}{r}\right)\\ &= 2M_j\left(-\boldsymbol{P}^2(\boldsymbol{Q}\cdot\boldsymbol{P}) + (\boldsymbol{P}\cdot\boldsymbol{Q})\boldsymbol{P}^2 + \frac{\alpha}{r}(\boldsymbol{Q}\cdot\boldsymbol{P}) - (\boldsymbol{P}\cdot\boldsymbol{Q})\frac{\alpha}{r}\right)\\ &= -2i\hbar M_j\left(\boldsymbol{P}^2 - \frac{2\alpha}{r}\right) = -4i\hbar M_jH,\end{aligned}$$

where we have used $[\boldsymbol{M}, \boldsymbol{P}\cdot\boldsymbol{Q}] = 0$ and $\left[\boldsymbol{P}\cdot\boldsymbol{Q}, \frac{1}{r}\right] = \frac{i\hbar}{r}$. This proves that $[W_k, W_l] = -2i\hbar\varepsilon_{jkl}M_jH$.

Let $\mathscr{H}_0 = \mathrm{P}_H(-\infty, 0)\mathscr{H}$, where P_H is the projection-valued measure for the Schrodinger operator H. Since self-adjoint operators M and W commute with H, the subspace $\mathscr{H}_0$ is an invariant subspace for these operators. The Schrodinger operator H is non-negative on $\mathscr{H}_0$, so that on this subspace the operator $(-2H)^{-1/2}$ is well defined. Now on $\mathscr{H}_0$ we set

$$\boldsymbol{J}^{(\pm)} = \frac{1}{2}\left(\boldsymbol{M} \pm (-2H)^{-1/2}W\right).$$

It follows from Proposition 5.1 that self-adjoint operators $J_j^{(\pm)}$on $\mathscr{H}_0$ satisfy the commutation relations

$$\left[J_j^{(\pm)}, J_k^{(\pm)}\right] = i\hbar\varepsilon_{jkl}J_l^{(\pm)}, \quad \left[J_j^{(+)}, J_k^{(-)}\right] = 0 \tag{5.21}$$

and

$$\left(\boldsymbol{J}^{(+)}\right)^2 = \left(\boldsymbol{J}^{(-)}\right)^2 = -\frac{1}{4}\left(\hbar^2 I + \frac{\alpha^2}{2H}\right). \tag{5.22}$$

Equations (5.21) are commutation relations for the generators of the Lie algebra $\mathfrak{so}(4)$, which correspond to the Lie isomorphism $\mathfrak{so}(4) \simeq \mathfrak{so}(3) \oplus \mathfrak{so}(3)$, and exhibit the hidden SO(4) symmetry of the Coulomb problem! Together with (5.22), they allow us to find the energy levels pure algebraically.

Namely, the eigenvalues of the operators $\left(\boldsymbol{J}^{(+)}\right)^2$ and $\left(\boldsymbol{J}^{(-)}\right)^2$ are, respectively, $\hbar^2 l_1\left(l_1+1\right)$ and $\hbar^2 l_2\left(l_2+1\right)$, and it follows from (5.22) that $l_1 = l_2 = l$ so that the corresponding eigenvalue of H is

$$E_n = -\frac{\alpha^2}{2\hbar^2 n^2}, \quad n = 2l+1$$

Assuming that

$$\mathscr{H}_0 \simeq \bigoplus_{l\in\frac{1}{2}\mathbb{Z}_{\geq 0}} V_l \otimes V_l \tag{5.23}$$

where summation goes over all non-negative integer and half-integer values of l, we get from the Clebsch-Gordan decomposition (3.13) that the multiplicity of the eigenvalue E_n is

$$\dim V_l \otimes V_l = \sum_{j=0}^{2l}(2j+1) = (2l+1)^2 = n^2$$

To prove the orthogonal sum decomposition (5.23), one should consider the Schrodinger equation for the hydrogen atom in the momentum representation. Using spherical coordinates in $\mathbb{R}^3$ and the elementary integral

$$\int_0^\infty \frac{\sin r}{r} dr = \frac{\pi}{2}$$

it is easy to show that for every $\psi \in \mathscr{S}\left(\mathbb{R}^3\right)$

$$\frac{1}{2\pi^2\hbar}\int_{\mathbb{R}^3}\frac{\hat{\psi}(\boldsymbol{q})}{|\boldsymbol{p}-\boldsymbol{q}|^2}d^3\boldsymbol{q} = \frac{1}{(\sqrt{2\pi\hbar})^3}\int_{\mathbb{R}^3}\frac{1}{r}\psi(\boldsymbol{x})e^{-\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{x}}d^3\boldsymbol{x} \tag{5.24}$$

where $\hat{\psi} = \mathscr{F}_\hbar(\psi)$ is the $\hbar$-dependent Fourier transform [9]. Let ψ be the eigenfunction of H with the the eigenvalue $E < 0$. It follows from (5.24) that in the momentum representation the corresponding Schrodinger equation the eigenvalue equation $H\psi = E\psi$ - takes the form

$$\left(\boldsymbol{p}^2 + p_0^2\right)\hat{\psi}(\boldsymbol{p}) = \lambda\int_{\mathbb{R}^3}\frac{\hat{\psi}(\boldsymbol{q})}{|\boldsymbol{p}-\boldsymbol{q}|^2}d^3\boldsymbol{q} \tag{5.25}$$

where $p_0 = \sqrt{-2\mu E}$ and $\lambda = \frac{\alpha\mu}{p_0\hbar}$. Next, consider the homogeneous coordinates $\frac{\boldsymbol{p}}{p_0}$ in $\mathbb{R}^3$ as coordinates of the stereographic projection of the unit sphere S^3 in $\mathbb{R}^4$. Namely, denoting by $\boldsymbol{n}$ the unit vector from the origin to the north pole of S^3, we get for the point $\boldsymbol{u} \in S^3$ corresponding to $\frac{\boldsymbol{p}}{p_0} \in \mathbb{R}^3$:

$$\boldsymbol{u} = \frac{\boldsymbol{p}^2 - p_0^2}{\boldsymbol{p}^2 + p_0^2}\boldsymbol{n} + \frac{2p_0}{\boldsymbol{p}^2 + p_0^2}\boldsymbol{p}$$

For the volume form on S^3 we have

$$d\Omega = \frac{(2p_0)^3}{(\boldsymbol{p}^2+p_0^2)^3}d^3\boldsymbol{p}, \quad \int_{S^3} d\Omega = 2\pi^2$$

Using

$$|\boldsymbol{p}-\boldsymbol{q}|^2 = \frac{(\boldsymbol{p}^2+p_0^2)\,(\boldsymbol{q}^2+p_0^2)}{(2p_0)^2}|\boldsymbol{u}-\boldsymbol{v}|^2$$

where $\boldsymbol{v}\in S^3$ corresponds to $\frac{\boldsymbol{q}}{p_0}\in\mathbb{R}^3$, and introducing

$$\Psi(\boldsymbol{u}) = \frac{1}{\sqrt{p_0}}\frac{(\boldsymbol{p}^2+p_0^2)^2}{(2p_0)^2}\hat{\psi}(\boldsymbol{p})$$

we can rewrite equation (5.25) as

$$\Psi(\boldsymbol{u}) = \frac{\lambda}{2\pi^2}\int_{S^3}\frac{\Psi(\boldsymbol{v})}{|\boldsymbol{u}-\boldsymbol{v}|^2}d\Omega_{\boldsymbol{v}} \tag{5.26}$$

We also have

$$\int_{S^3}|\Psi(\boldsymbol{u})|^2 d\Omega_{\boldsymbol{u}} = \int_{\mathbb{R}^3}\frac{\boldsymbol{p}^2+p_0^2}{2p_0^2}|\hat{\psi}(\boldsymbol{p})|^2 d^3\boldsymbol{p} = \int_{\mathbb{R}^3}|\hat{\psi}(\boldsymbol{p})|^2 d^3\boldsymbol{p}. \tag{5.27}$$

Indeed, it follows from the Schrodinger equation that

$$\frac{1}{2\mu}\int_{\mathbb{R}^3}\boldsymbol{p}^2|\hat{\psi}(\boldsymbol{p})|^2 d^3\boldsymbol{p} = \frac{1}{2\mu}\int_{\mathbb{R}^3}\left|\frac{\partial\psi(\boldsymbol{x})}{\partial\boldsymbol{x}}\right|^2 d^3\boldsymbol{x} = \int_{\mathbb{R}^3}(E-V(r))|\psi(\boldsymbol{x})|^2 d^3\boldsymbol{x},$$

and by the virial theorem (see Section 1.3) we get
$\frac{1}{2\mu}\int_{\mathbb{R}^3}\left|\frac{\partial\psi(\boldsymbol{x})}{\partial\boldsymbol{x}}\right|^2 d^3\boldsymbol{x} = -\frac{1}{2\mu}\int_{\mathbb{R}^3}\Delta\psi(\boldsymbol{x})\overline{\psi(\boldsymbol{x})}d^3\boldsymbol{x} = -\frac{1}{2}\int_{\mathbb{R}^3}V(r)|\psi(\boldsymbol{x})|^2 d^3\boldsymbol{x}$, where $V(r) = -\frac{\alpha}{r}$, so that

$$\int_{\mathbb{R}^3}V(r)|\psi(\boldsymbol{x})|^2 d^3\boldsymbol{x} = 2E\int_{\mathbb{R}^3}|\psi(\boldsymbol{x})|^2 d^3\boldsymbol{x} = 2E\int_{\mathbb{R}^3}|\hat{\psi}(\boldsymbol{p})|^2 d^3\boldsymbol{p}.$$

This shows that the eigenvalue problem for the Schrodinger equation is equivalent to the eigenvalue problem for the integral equation (5.26) in $L^2(S^3, d\Omega)$. The latter is a classical problem in the theory of spherical harmonics. Namely, the function $G(\boldsymbol{u}) = -\frac{1}{4\pi^2 u^2}$, where $u = |\boldsymbol{u}|, \boldsymbol{u}\in\mathbb{R}^4$, is the fundamental solution for the Laplace operator Δ in $\mathbb{R}^4$,

$$\Delta = \frac{\partial^2}{\partial u_1^2}+\frac{\partial^2}{\partial u_2^2}+\frac{\partial^2}{\partial u_3^2}+\frac{\partial^2}{\partial u_4^2},$$

and equation (5.26) is the equation satisfied by the spherical harmonics on S^3: the eigenfunctions of the spherical part Δ_0 of the Laplace operator on $\mathbb{R}^4$, defined by

$$\Delta = \frac{1}{u^3}\frac{\partial}{\partial u}\left(u^3\frac{\partial}{\partial u}\right)+\frac{1}{u^2}\Delta_0.$$

It is well known from the representation theory of the Lie group SO(4) that spherical harmonics are restrictions to S^3 of homogeneous harmonic polynomials in $\mathbb{R}^4$ of degree $n-1, n\in$

[09] Since $\boldsymbol{x}$ is the variable in the coordinate representation, here $\boldsymbol{q}$ is another variable in the momentum representation.

$\mathbb{N}$. Correspondingly, equation (5.26) is obtained as a limit $|\boldsymbol{u}| \to 1$ of the Green's formula for the homogeneous harmonic function of degree $n-1$ in the unit ball in $\mathbb{R}^4$, by using the property of a double layer potential. This gives $\lambda = n$, which once again establishes the exact formula for the energy levels of the hydrogen atom. The isomorphism $\mathscr{H}_0 \simeq L^2(S^3, d\Omega)$ follows from (5.27), and (5.23) - from the decomposition

$$L^2\left(S^3, d\Omega\right) \simeq \bigoplus_{l \in \frac{1}{2}\mathbb{Z}_{\geq 0}} V_l \otimes V_l$$

of the regular representation of SO(4) into the direct sum of irreducible components. One can also obtain the explicit form (5.4) of the eigenfunctions by using the representation theory of SO(4). We leave all these details to the interested reader.

Remark. For $E > 0$ one should consider the subspace $\mathscr{H}_1 = \mathrm{P}_H(0,\infty)\mathscr{H}$ and define $\boldsymbol{J}^{(\pm)} = \frac{1}{2}\left(\boldsymbol{M} \pm (2H)^{-1/2}\boldsymbol{W}\right)$. Instead of (5.21), these operators satisfy commutation relations of the Lie algebra $\mathfrak{so}(3,1)$ of the Lorentz group SO(3,1). The problem of finding eigenfunctions of the continuous spectrum for the Coulomb problem can be solved by using harmonic analysis on the three-dimensional Lobachevsky space.

Problem 5.1. Show that components of angular momentum M are generators of $\mathfrak{so}(4)$ that correspond to the infinitesimal rotations in the subspace of $\mathbb{R}^4$ with coordinates $(0, \boldsymbol{p})$, and components of the Laplace-Runge-Lenz vector $\boldsymbol{W}$ correspond to the infinitesimal rotations in the $(p_0 p_1), (p_0, p_2)$, and $(p_0 p_3)$ planes in $\mathbb{R}^4$.

3.6.12 6. Semi-classical asymptotics - I

Theory

Here we describe the relation between classical and quantum mechanics by considering the behavior of the wave function $\psi(\boldsymbol{q}, t)$ - the solution of the time dependent Schrodinger equation [10]

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + V(\boldsymbol{q})\psi \tag{6.1}$$

as $\hbar \to 0$. The substitution

$$\psi(\boldsymbol{q}, t) = e^{-\frac{i}{\hbar}S(\boldsymbol{q},t;\hbar)} \tag{6.2}$$

reduces (6.1) to the following non-linear partial differential equation:

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial \boldsymbol{q}}\right)^2 + V(\boldsymbol{q}) = \frac{i\hbar}{2m}\Delta S \tag{6.3}$$

It is remarkable that (6.3) differs from the Hamilton-Jacobi equation (2.4) for the Hamiltonian function $H_c(\boldsymbol{p}, \boldsymbol{q}) = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{q})$, considered in Section 2.3 of Chapter 1, only by the term in the right-hand side which is proportional to $\hbar$. Thus as $\hbar \to 0$, equations of motion in quantum mechanics turn into classical equations of motion.

For the stationary state $\psi(\boldsymbol{q}, t) = \psi(\boldsymbol{q})e^{-\frac{i}{\hbar}Et}$ the substitution (6.2) becomes

$$\psi(\boldsymbol{q}, t) = e^{-\frac{i}{\hbar}(\sigma(\boldsymbol{q};\hbar) - Et)}. \tag{6.4}$$

The corresponding non-linear partial differential equation

[10] Here it is convenient to denote Cartesian coordinates on $\mathbb{R}^n$ by $\boldsymbol{q} = (q_1, ..., q_n)$.

$$\frac{1}{2m}\left(\frac{\partial\sigma}{\partial \boldsymbol{q}}\right)^2 + V(\boldsymbol{q}) = E + \frac{i\hbar}{2m}\Delta\sigma \tag{6.5}$$

differs from the corresponding Hamilton-Jacobi equation for the abbreviated action, considered in Section 2.5 of Chapter 1, by the term proportional to $\hbar$ in the right-hand side.

In this section we consider semi-classical asymptotics: asymptotics of the partial differential equations (6.3) and (6.5) as $\hbar \to 0$. They describe the precise relation between quantum mechanics and classical mechanics, and provide a quantitative form of the correspondence principle, discussed in Section 2 of Chapter 2. In particular, using semi-classical asymptotics for the stationary Schrodinger equation, we derive Bohr-Wilson-Sommerfeld quantization rules, postulated in Section 2.5 of Chapter 2.

6.1. Time-dependent asymptotics.

Here we consider the problem of finding short-wave asymptotics - asymptotics as $\hbar \to 0$ of the solution $\psi_\hbar(q,t)$ of the Cauchy problem for the Schrodinger equation (6.1) in one dimension,

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial q^2} + V(q)\psi$$

with the initial condition

$$\psi_\hbar(q,t)|_{t=0} = \varphi(q)e^{\frac{i}{\hbar}s(q)}.$$

It is assumed that the real-valued functions $\varphi(q)$ and $s(q)$ are smooth, $s(q), \varphi(q) \in C^\infty(\mathbb{R})$, and that the "amplitude" $\varphi(q)$ has compact support. The substitution (6.2) is $\psi_\hbar(q,t) = e^{\frac{i}{\hbar}S(q,t,\hbar)}$, and differential equation (6.3) takes the form

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial q}\right)^2 + V(q) = \frac{i\hbar}{2m}\frac{\partial^2 S}{\partial q^2}. \tag{6.6}$$

To determine the asymptotic behavior of $S(q,t,\hbar)$ as $\hbar \to 0$, we assume that as $\hbar \to 0$

$$S(q,t,\hbar) = \sum_{n=0}^{\infty}(-i\hbar)^n S_n(q,t),$$

and substitute this expansion into (6.6). Comparing terms with the same powers of $\hbar$ we obtain that $S_0(q,t)$ satisfies the initial value problem

$$\frac{\partial S_0}{\partial t} + \frac{1}{2m}\left(\frac{\partial S_0}{\partial q}\right)^2 + V(q) = 0 \tag{6.7}$$

and

$$S_0(q,t)|_{t=0} = s(q) \tag{6.8}$$

whereas $S_1(q,t)$ satisfies the differential equation

$$\frac{\partial S_1}{\partial t} + \frac{1}{m}\frac{\partial S_0}{\partial q}\frac{\partial S_1}{\partial q} = -\frac{1}{2m}\frac{\partial^2 S_0}{\partial q^2} \tag{6.9}$$

the so-called transport equation, and

$$S_1(q,t)|_{t=0} = \varphi(q) \tag{6.10}$$

The functions $S_n(q,t)$ for $n > 1$ satisfy non-homogeneous differential equations similar to (6.9).

The initial value problem (6.7)-(6.8) is the Cauchy problem for the Hamilton-Jacobi equation with the Hamiltonian function

$$H_{\mathrm{c}}(p,q) = \frac{p^2}{2m} + V(q)$$

considered in Section 2.3 of Chapter 1. According to Proposition 2.1 in Section 2.3 of Chapter 1, the solution of (6.7)-(6.8) is given by the method of characteristics,

$$S_0(q,t) = s\left(q_0\right) + \int_0^t L\left(\gamma'(\tau)\right) d\tau \tag{6.11}$$

Here $L(q,\dot{q}) = \frac{1}{2}m\dot{q}^2 - V(q)$ is the Lagrangian function, and $\gamma(\tau)$ is the characteristic - the classical trajectory which starts at q_0 at time $\tau = 0$ with the momentum $p_0 = \frac{\partial s}{\partial q}\left(q_0\right)$, and ends at q at time $\tau = t$, where q_0 is uniquely determined by q. (We are assuming that the Hamiltonian phase flow g_t satisfies the assumptions made in Section 2.3 of Chapter 1.) It follows from Theorem 2.7 in Section 2.3 of Chapter 1 that along the characteristic,

$$\frac{\partial S_0}{\partial q}(q,t) = m\frac{d\gamma}{dt}(t)$$

so that

$$\left(\frac{\partial}{\partial t} + \frac{\partial S_0}{\partial q}\right) S_1(\gamma(t),t) = \frac{d}{dt} S_1(\gamma(t),t) \tag{6.12}$$

Now we can solve the Cauchy problem (6.9)-(6.10) for the transport equation explicitly. Consider the flow $\pi_t : \mathbb{R} \to \mathbb{R}$, defined in Section 2.3 of

Chapter 1, and denote [11] by $\gamma(Q,q;\tau)$ the characteristic connecting points q at $\tau = 0$ and $Q = \pi^t(q)$ at $\tau = t$ (under our assumptions the flow π_t is a diffeomorphism and the mapping $q \mapsto Q$ is one to one). Differentiating the equation

$$\frac{\partial S_0}{\partial Q}(Q,t) = m\frac{\partial \gamma}{\partial t}(Q,q;t)$$

with respect to q we obtain

$$\frac{\partial^2 S_0}{\partial Q^2}(Q,t)\frac{\partial Q}{\partial q} = m\frac{\partial^2 \gamma}{\partial q \partial t}(Q,q;t) = m\frac{d}{dt}\left(\frac{\partial Q}{\partial q}\right)$$

so that (6.9) can be rewritten as

$$\frac{d}{dt} S_1(Q,t) = -\frac{1}{2}\frac{d}{dt}\log\frac{\partial Q}{\partial q}$$

and using (6.10) we obtain

$$S_1(Q,t) = \varphi(q)\left|\frac{\partial Q}{\partial q}(q)\right|^{-\frac{1}{2}}$$

Therefore,

$$\psi_\hbar(Q,t) = \varphi(q)\left|\frac{\partial Q}{\partial q}(q)\right|^{-\frac{1}{2}} e^{\frac{i}{\hbar}(S(Q,q;t)+s(q))}(1+O(\hbar)) \tag{6.13}$$

where $S(Q,q;t)$ is the classical action along the characteristic that starts at q at time $\tau=0$ and ends at Q at time $\tau=t$.

The rigorous proof that (6.13) is an asymptotic expansion as $\hbar\to 0$ uses the assumptions made in Section 2.3 of Chapter 1, and is left to the interested reader. Here we just mention that asymptotics (6.13) is consistent with the conservation of probability: for any Borel subset $E\subset\mathbb{R}$,

$$\int_{E_t}|\psi_\hbar(Q,t)|^2\,dQ=\int_E|\varphi(q)|^2dq+O(\hbar)$$

as $\hbar\to 0$, where $E_t=\pi_t(E)$.

Remark. When assumptions in Section 2.3 of Chapter 1 are not satisfied, the situation becomes more complicated. Namely, in this case there may be several characteristics $\gamma_j(\tau)$ which end at Q at $\tau=t$ having q_j as their corresponding initial points. In this case,

$$\psi_\hbar(Q,t)=\sum_j\varphi\left(q_j\right)\left|\frac{\partial Q}{\partial q}\left(q_j\right)\right|^{-\frac12}e^{\frac{i}{\hbar}(S(Q,q_j;t)+s(q_j))-\frac{\pi i}{2}\mu_j}(1+O(\hbar))$$

where $\mu_j\in\mathbb{Z}$ is the Morse index of the characteristic γ_j. It is defined as the number of focal points of the phase curve $(q(\tau),p(\tau))$ with initial data

q_j and $p_j=\frac{\partial s}{\partial q}\left(q_j\right)$ with respect to the configuration space $\mathbb{R}$. It is a special case of a more general Maslov index.

The case of n degrees of freedom is considered similarly. Under the assumptions in Section 2.3 of Chapter 1, the solution $\psi_\hbar(\boldsymbol{q},t)$ of the Schrodinger equation (6.1) with the initial condition

$$\psi_\hbar(\boldsymbol{q},t)|_{t=0}=\varphi(\boldsymbol{q})e^{\frac{i}{\hbar}s(\boldsymbol{q})}$$

where real-valued functions $s(\boldsymbol{q})$ and $\varphi(\boldsymbol{q})$ are smooth and $\varphi(\boldsymbol{q})$ is compactly supported, has the following asymptotics as $\hbar\to 0$:

$$\psi_\hbar(\boldsymbol{Q},t)=\varphi(\boldsymbol{q})\left|\det\left(\frac{\partial\boldsymbol{Q}}{\partial\boldsymbol{q}}(\boldsymbol{q})\right)\right|^{-\frac12}e^{\frac{i}{\hbar}(S(\boldsymbol{Q},\boldsymbol{q};t)+s(\boldsymbol{q}))}(1+O(\hbar)).\tag{6.14}$$

6.2. Time independent asymptotics. Here we consider semi-classical asymptotics for the one-dimensional Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi\tag{6.15}$$

This asymptotic method is also known as the WKB method (after G. Wentzel, H. Kramers, and L. Brillouin). The substitution (6.4) is $\psi_\hbar(x)=e^{\frac{i}{\hbar}\sigma(x;\hbar)}$ and equation (6.5) takes the form

$$\frac{1}{2m}\left(\frac{d\sigma}{dx}\right)^2+V(x)=E+\frac{i\hbar}{2m}\frac{d^2\sigma}{dx^2}$$

As in the previous section, we use the expansion

$$\sigma(x,\hbar)=\sum_{n=0}^{\infty}(-i\hbar)^n\sigma_n(x)$$

and for the first two terms obtain

$$\frac{1}{2m}\sigma_0'^2=E-V(x)\quad\text{ and }\quad\sigma_0'\sigma_1'=-\frac12\sigma_0''.\tag{6.16}$$

[011] There should not be any confusion with the quantum coordinate operator Q.

Let $p(x) = \sqrt{2m(E - V(x))}$ be the classical momentum of a particle moving in a potential $V(x)$ with the energy E. The solution of the first equation in (6.16) is given by

$$\sigma_0 = \pm \int p(x)dx$$

and from the second equation in (6.16) we get

$$\sigma_1 = -\frac{1}{2}\log p$$

The wave function in the WKB approximation has the form

$$\psi_\hbar(x) = \frac{1}{\sqrt{|p(x)|}}\left(C_1 e^{\frac{i}{\hbar}\int p(x)dx} + C_2 e^{-\frac{i}{\hbar}\int p(x)dx}\right)(1 + O(\hbar)), \tag{6.17}$$

where $p(x)$ is real in the classical region $V(x) < E$, and is pure imaginary in the classically forbidden region $V(x) > E$ (see Section 1.5 of Chapter 1).

Note that the asymptotic (6.17) is valid only if $\sigma^2 \ll \hbar\sigma''$, which in the first approximation gives

$$\left|\frac{d}{dx}\left(\frac{\hbar}{p(x)}\right)\right| \ll 1.$$

Introducing the classical force $F = -\frac{dV}{dx}$, this condition can be written as

$$\frac{m\hbar F}{p^3} \ll 1 \tag{6.18}$$

Thus the WKB approximation does not work when the classical momentum $p(x)$ is small. In particular, it is not applicable near the turning points where $E = V(x)$ and, therefore, $p(x) = 0$. Let $x = a$ be a turning point. If $F_0 = F(a) \neq 0$, using the approximation $E - V(x) \simeq F_0(x - a)$ near $x = a$, one can replace (6.15) by

$$\frac{\hbar^2}{2m}\psi'' = F_0(x - a)\psi$$

This differential equation can be explicitly solved by the Laplace method. Its bounded solution is

$$\psi(x) = \Phi(\xi), \quad \xi = \left(\frac{2mF_0}{\hbar^2}\right)^{\frac{1}{3}}(a - x)$$

where $\Phi(\xi)$ is the Airy-Fock function, defined by the improper integral

$$\Phi(\xi) = \frac{1}{\sqrt{\pi}}\int_0^\infty \cos\left(\frac{1}{3}t^3 + \xi t\right)dt.$$

The large ξ asymptotics of the Airy-Fock function, obtained by the steepest descent method, are the following:

$$\Phi(\xi) = \frac{1}{2\sqrt[4]{\xi}}e^{-\frac{2}{3}\xi^{\frac{3}{2}}}\left(1 + O\left(\xi^{-\frac{3}{2}}\right)\right) \quad \text{as} \quad \xi \to \infty, \tag{6.19}$$

$$\Phi(\xi) = \frac{1}{\sqrt[4]{|\xi|}}\sin\left(\frac{2}{3}|\xi|^{\frac{3}{2}} + \frac{\pi}{4}\right)\left(1 + O\left(|\xi|^{-\frac{3}{2}}\right)\right) \quad \text{as} \quad \xi \to -\infty. \tag{6.20}$$

Using asymptotics (6.19)-(6.20) one can obtain connection formulas relating WKB approximations for classical and forbidden regions. The rigorous justification of this approach is technically rather involved and we will not present it here. Instead we highlight the simplest case when there is only one turning point $x = a$ with $F_0 > 0$, so that $x < a$ is a classically forbidden region. From (6.17) we obtain that the WKB wave function in the forbidden region $x < a$ is exponentially decaying,

$$\psi_{\mathrm{WKB}}(x) = \frac{A}{\sqrt{|p(x)|}} e^{\frac{1}{\hbar}\int_a^x |p(s)|ds},$$

whereas in the classical region $x < a$ it is oscillating, $\psi_{\mathrm{WKB}}(x) = \frac{1}{\sqrt{p(x)}}\left(C_1 e^{\frac{i}{\hbar}\int_a^x p(s)ds} + C_2 e^{-\frac{i}{\hbar}\int_a^x p(s)ds}\right) = \frac{B}{\sqrt{p(x)}}\sin\left(\frac{1}{\hbar}\int_a^x p(s)ds + \alpha\right)$.
As follows from (6.18), the WKB approximation near the turning point $x = a$ remains valid whenever $|x-a| \gg \frac{1}{2}\left(\frac{\hbar^2}{mF_0}\right)^{\frac{1}{3}}$, which is equivalent to the condition $|\xi| \gg 1$. On the other hand, when $|x-a| \ll 1$ the wave function has the asymptotic

$$\psi_\hbar(x) = C\Phi(\xi)(1 + O(\hbar))$$

To determine the unknown phase α and to find the relation between coefficients A, B, and C, we consider the domain $\frac{1}{2}\left(\frac{\hbar^2}{mF_0}\right)^{\frac{1}{3}} \ll |x-a| \ll 1$ and compare the WKB approximation for the wave function with the large ξ asymptotics of the Airy-Fock function. Namely, for $x < a$ we have $\xi \gg 1$ and

$$\frac{2}{3}\xi^{\frac{3}{2}} = \frac{2}{3\hbar}\sqrt{2mF_0}(a-x)^{\frac{3}{2}} \simeq \frac{1}{\hbar}\int_x^a |p(s)|ds, \quad \sqrt[4]{\xi} = \frac{\sqrt{|p(x)|}}{\sqrt[6]{2m\hbar F_0}}$$

Comparing (6.19) with the WKB wave function for $x < a$ we obtain that $2A = \sqrt[6]{2m\hbar F_0}C$. For $x > a$ we have $\xi \ll -1$ and

$$\frac{2}{3}|\xi|^{\frac{3}{2}} = \frac{2}{3\hbar}\sqrt{2mF_0}(x-a)^{\frac{3}{2}} \simeq \frac{1}{\hbar}\int_a^x p(s)ds, \quad \sqrt[4]{|\xi|} = \frac{\sqrt{p(x)}}{\sqrt[6]{2m\hbar F_0}}$$

Comparing (6.20) with the WKB wave function for $x < a$ we obtain that $\alpha = \frac{\pi}{4}$ and $B = \sqrt[6]{2m\hbar\overline{F_0}}C$, so that $B = 2A$. Thus for this example the WKB wave function is

$$\psi_{\mathrm{WKB}}(x) = \begin{cases} \frac{A}{\sqrt{|p(x)|}} e^{\frac{1}{\hbar}\int_a^x |p(s)|ds} & \text{when } x < a \\ \frac{2A}{\sqrt{p(x)}}\sin\left(\frac{1}{\hbar}\int_a^x p(s)ds + \frac{\pi}{4}\right) & \text{when } x > a \end{cases} \tag{6.21}$$

The case when there is only one turning point $x = b$ with $F_0 < 0$, so that $x > b$ is a classically forbidden region, reduces to the previous example by reversing the orientation $x \mapsto -x$. As the result, we obtain

$$\psi_{\mathrm{WKB}}(x) = \begin{cases} \frac{2B}{\sqrt{p(x)}}\sin\left(\frac{1}{\hbar}\int_x^b p(s)ds + \frac{\pi}{4}\right) & \text{when } x < b \\ \frac{B}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_b^x |p(s)|ds} & \text{when } x > b \end{cases} \tag{6.22}$$

Problem 6.1 (Penetration through a potential barrier). Consider a potential barrier for a given energy E - a potential $V(x)$ such that $\{x \in \mathbb{R} : V(x) > E\} = (a, b)$. Show that

$$T_{\mathrm{WKB}} = e^{-\frac{2}{\hbar}\int_a^b |p(x)|dx}.$$

Verify directly that transmission coefficient for the potential in Problem 2.9 in the semi-classical approximation is given by this formula.

Problem 6.2 (Above barrier reflection). Suppose that a potential $V(x)$ admits analytic continuation into the upper half-plane, and let E be the energy such that $E > V(x)$ for all real x. Suppose that there is only one complex x_0 such that $V(x_0) = E$. Show that in the semi-classical approximation

$$R_{\mathrm{WKB}} = e^{-\frac{4}{\hbar}\operatorname{Im}\int_a^{x0} p(x)dx},$$

where $p(x) = \sqrt{2m(E - V(x))}$ and $a \in \mathbb{R}$ (the choice of a does not change the imaginary part of the integral in the exponent). Verify directly that the reflection coefficient for the potential in Problem 2.9 in the semi-classical approximation is given by this formula.

Problem 6.3. Find transmission and reflection coefficients for the parabolic barrier - a potential $V(x) = -\frac{1}{2}kx^2$, where $k > 0$ - and verify directly that in the semi-classical approximation they satisfy, for $E < 0$ and $E > 0$, respectively, formulas in Problems 6.1 and 6.2.

6.3. Bohr-Wilson-Sommerfeld quantization rules. The WKB method allows us to determine energy levels in the semi-classical approximation. Consider, for simplicity, the finite motion of a one-dimensional particle in a potential well: in a potential $V(x)$ at the energy E such that there are two turning points a and b. The classical region is $a \le x \le b$, and the motion is periodic with the period

$$T = 2\int_a^b \frac{dx}{\dot{x}} = 2m\int_a^b \frac{dx}{p} = \sqrt{2m}\int_a^b \frac{dx}{\sqrt{E - V(x)}}.$$

The regions $x < a$ and $x > b$ are forbidden (see Section 1.5 of Chapter 1).

It follows from (6.21)-(6.22) that the WKB wave function exponentially decays in the forbidden regions $x < a$ and $x > b$. Using (6.21) we see that in the classical region the WKB wave function has the form

$$\psi_{\mathrm{WKB}}(x) = \frac{2A}{\sqrt{p(x)}}\sin\left(\frac{1}{\hbar}\int_a^x p(s)ds + \frac{\pi}{4}\right),$$

while using (6.22) we obtain

$$\begin{aligned}\psi_{\mathrm{WKB}}(x) &= \frac{2B}{\sqrt{p(x)}}\sin\left(\frac{1}{\hbar}\int_x^b p(s)ds + \frac{\pi}{4}\right)\\ &= \frac{2B}{\sqrt{p(x)}}\sin\left(\frac{1}{\hbar}\int_a^b p(s)ds + \frac{\pi}{2} - \left(\frac{1}{\hbar}\int_a^x p(s)ds + \frac{\pi}{4}\right)\right).\end{aligned}$$

These two expressions define the same function in $a \le x \le b$ if and only if there is a positive integer n such that

$$\frac{1}{\hbar}\int_a^b p(x)dx + \frac{\pi}{2} = (n+1)\pi, \tag{6.23}$$

in which case $A = (-1)^{n+1}B$. Equation (6.23), written in the form

$$\int_a^b \sqrt{2m(E - V(x))}dx = \pi\hbar\left(n + \frac{1}{2}\right)$$

determines the semi-classical energy levels. It follows from (6.21)-(6.22) that the integer n is equal to the number of zeros of the WKB wave function. In accordance with the oscillation theorem, the case $n = 0$ corresponds to the ground state, case $n = 1$ - to the next energy level state, etc.

Denoting, as in Chapters 1 and 2, coordinate x by q, we can rewrite (6.23) as

$$\oint p dq = 2\pi\hbar \left(n + \frac{1}{2}\right), \tag{6.24}$$

where integration goes over the closed classical orbit in the phase plane $\mathbb{R}^2$ with canonical coordinates p, q. Condition (6.24) is the famous Bohr-Wilson-Sommerfeld quantization rule for the case of one degree of freedom (see Section 2.5 of Chapter 2). We emphasize that, in general, the BWS quantization rule is applicable only for large n and gives the semi-classical asymptotic of energy levels E_n. However, as was shown in Section 2.6 of Chapter 2, the energy levels of the harmonic oscillator obtained by the BWS quantization rule are exact. The BWS rules are also exact for the energy levels of the hydrogen atom (see Section 5.1).

This semi-classical analysis can be generalized for quantum systems with n degrees of freedom which correspond to completely integrable classical Hamiltonian systems (see Section 2.6 of Chapter 1). Bohr-WilsonSommerfeld quantization rules take the form

$$\oint_\gamma \boldsymbol{p} d\boldsymbol{q} = 2\pi\hbar \left(n_\gamma + \frac{1}{4} \text{ ind } \gamma\right). \tag{6.25}$$

Here integration goes over all 1-cycles γ in the Lagrangian submanifold $\Lambda = \{(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{R}^{2n} : H_c(\boldsymbol{p}, \boldsymbol{q}) = E, F_2(\boldsymbol{p}, \boldsymbol{q}) = E_2, ..., F_n(\boldsymbol{p}, \boldsymbol{q}) = E_n\}$, and ind γ is the Maslov index of a cycle γ in Λ. For the action-angle variables $(\boldsymbol{I}, \boldsymbol{\varphi})$ the integration in (6.25) goes over the basic 1 -cycles on the n-torus T^n, and we obtain quantization conditions $I_i = \left(n_i + \frac{1}{2}\right)\hbar, i = 1, ..., n$.

3.6.13 How to guess about Schrodinger equation?

(conceptually important question, but few people were really thinking about it beyond "we take Hamilton-Jacobi equation"... I'll think later. from which experiment? an answer to some question of early 19's)

3.6.14 Limits of Applicability of Schrodinger equation

(discussion in details, where it does not work?)

3.7 Heisenberg's Quantum Mechanics

Обзор форамлизма Гейзенберга

(тут будут ответы на все актуальные вопросы)

Мотивация изучать представление Гейзенберга

(я пока что не знаю, нафига оно нужно, но буду пользоваться - пропишу)

Об уравнении Гейзенберга

Уравнение Гейзенберга в двух словах

Представление Гейзенберга характерно тем, что в нем эволюционируют операторы, а не волновые функции.

отличие от Шредингера

применения

актуально увидеть, что конкретно им решается?

итоговые методы

Уравнение Гейзенберга для оператора $\hat{A}_H$ в представлении гейзенберга имеет вид:

$$\frac{d}{dt}\hat{A}_H(t) = \frac{i}{\hbar}\left[\hat{H}, \hat{A}_H(t)\right] + \frac{\partial \hat{A}_H}{\partial t}$$

Переход в представление гейзенберга происходит по средством оператора эволюции:

$$\hat{F}_H(t) = \hat{U}^\dagger(t)\hat{F}\hat{U}(t)$$

вывод уравнений и способа перехода в представление Гейзенберга

(все из киселева перепишу)

Рассмотрим матричный элемент произвольного оператора $\hat{F}$ в представлении Шредингера:

$$\langle \Phi(t)|F\Psi(t)\rangle = \langle U(t)\Phi|FU(t)\Psi\rangle = \left\langle \Phi|U^\dagger(t)FU(t)\Psi\right\rangle$$

Поэтому если волновую функцию рассматривать как неизменную величину, а единственным изменяющимся объектом были бы операторы, то их эволюция определялась бы:

$$\hat{F}_H(t) = \hat{U}^\dagger(t)\hat{F}\hat{U}(t)$$

Так и происходит переход в представление Гейзенберга.

Этот переход сохраняет эрмитовость, действительно:

$$\hat{F}^\dagger = \hat{F} \quad \leftrightarrow \quad \hat{F}_H^\dagger = \left(\hat{U}^\dagger\hat{F}\hat{U}\right)^\dagger = \hat{U}^\dagger\hat{F}\hat{U} = \hat{F}_H$$

Теперь получим уравнение динамики этих операторов.

Для этого продифференцируем оператор в представлении гейзенберга по времени и домножим на константы, чтобы воспользоваться уравнением Шредингера. Получим следующее:

$$\mathrm{i}\hbar\frac{d\hat{F}_H}{dt} = \mathrm{i}\hbar\hat{U}^\dagger\frac{\partial\hat{F}}{\partial t}\hat{U} + \hat{U}^\dagger(-\hat{H}\hat{F} + \hat{F}\hat{H})\hat{U}$$

Первый член правой части равен нулю, а второй с помощью $\hat{U}^\dagger\hat{U} = 1$ можно перевести в представление Гейзенберга:

$$\hat{U}^\dagger(-\hat{H}\hat{F} + \hat{F}\hat{H})\hat{U} = \left(\hat{U}^\dagger\hat{F}\hat{U}\right)\left(\hat{U}^\dagger\hat{H}U\right) - \left(U^\dagger\hat{H}\hat{U}\right)\left(U^\dagger\hat{F}\hat{U}\right) = \left[\hat{F}_H, \hat{H}_H\right]$$

В итоге уравнение динамики имеет вид:

$$\mathrm{i}\hbar\frac{dF}{dt} = [\hat{F}_H, \hat{H}_H]$$

Посмотрим далее на свойства этого уравнения.

матричная механика

Можно записать операторы и их уравнения в матричном виде:

$$\mathrm{i}\hbar\frac{dF_{nm}}{dt} = \left\langle n \left| \left[\hat{F}_H, \hat{H}_H\right] \right| m \right\rangle$$

Если наблюдаемая не зависит от времени явно, то можно взять матричный элемент по двум состояниям:

$$\mathrm{i}\hbar\frac{dF_{nm}}{dt} = \left\langle n\hat{F}_H, \hat{H}_H m \right\rangle$$

Преобразуем коммутатор

$$\left\langle n \left| \hat{F}_H \left(\sum_k |k\rangle\langle k| \right) \hat{H}_H - \hat{H}_H \left(\sum_k |k\rangle\langle k| \right) \hat{F}_H \right| m \right\rangle = \sum_k \left(F_{nk}H_{km} - H_{nk}F_{km}\right)$$

В итоге у нас появляется уравнение матричной механики:

$$\mathrm{i}\hbar\frac{dF_{nm}}{dt} = \sum_k \left(F_{nk}H_{km} - H_{nk}F_{km}\right)$$

Если система консервативна (?)б то базис строится по собственным функциям оператора $H_{km} = E_m\delta_{km}$, тогда уравнение гейзенберга будет иметь вид:

$$\mathrm{i}\hbar\frac{dF_{nm}}{dt} = F_{nm}\left(E_n - E_m\right)$$

пример решения хотя бы чего-то уравнением Гейзенберга

Киселев предлагает записать осциллятор в представлении Гейзенберга.

но после того, как он записал, он просто забил, так что я суть так и не понял, поэтому этот раздел откладывается на потом...

$$H(q,p) = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2} \quad \rightarrow \quad E_n = \frac{1}{2m}p_{nk}p_{kn} + \frac{m\omega^2}{2}q_{nk}q_{kn}$$

$$\langle n|[\hat{q},\hat{H}]|m\rangle = \left\langle n \left| \frac{\partial H}{\partial p} \right| m \right\rangle = \left\langle n \left| \frac{\hat{p}}{m} \right| m \right\rangle = \frac{p_{nm}}{m}$$

$$i\hbar\frac{dq_{nm}}{dt} = q_{nm}\left(E_n - E_m\right) = \frac{p_{nm}}{m}$$

соотношение неопределнностей энергии время

(тут - в качестве иллюстрации методы Гейзенберга, вообще подробно это будет написано в главе про соотношение неопределенностей, наверное, в научпопе)

(стр 43 киселев)

(место мотивации, зачем оно?)

$$[\hat{A},\hat{H}] = \mathrm{i}\hbar\frac{d\hat{A}}{dt}$$

$$\Delta A\Delta E \geqslant \frac{\hbar}{2}\left|\left\langle\frac{d\hat{A}}{dt}\right\rangle\right|$$

$$\left|\left\langle\frac{d\hat{A}}{dt}\right\rangle\right| = \frac{\Delta A}{\Delta t}$$

$$\Delta E\Delta t \geqslant \frac{\hbar}{2}$$

4 Other Fundamentals of Mathematical Quantum Mechanics

(later in this section, there will be a connection with quantum information theory)

4.1 Other, Fundamental Properties of Quantum Systems

4.1.1 Uncertainty Principle: Main Idea and Derivation

Обсудим подробно соотношение неопределенностей.

Соотношение неопределенностей для операторов в общем случае (??)

(тут страничка от Киселева про это)

Соотношение неопределенностей для энергии и времени (??)

(ну такая есть, и что??)

Connection of Fourier transformation and uncertainty principle in QM

(??? are they connected? I am not sure)

О неверных пониманиях соотношения неопределенностей (??)

(??? what can be and what can't be??? these are the important questions)

Соотношение неопределенностей для операторов в общем случае (??)

О применениях соотношения неопределенностей (??)

(тоже сразу укажу, где она нужна, а где нет.)

Об экспериментальной проверке соотношения неопределенностей (???)

(как конкретно проверить, что оно на самом деле есть? хз.)

Uncertainty in Fourier transformation

Does uncertainty principle have something to do with experiment

We were taught that no, we can derive it from theory. But there should be some further experimental restrictions!
(????)
(discuss!!!)

4.1.2 Uncertainty Principle: Other Questions

(maybe I'll create a section for each paragraph here later)

Connection of uncertainty principle and other quantum laws

(a big general question)

Соотношение неопределенностей энергия-время

Обсудим подробно соотношение неопределенностей энергия-время.
(думаю, это заслуживает отдельного раздела, тут много сложностей)

Experimental Confirmation of Uncertainty Principle

(??? I'll read something about it later)

How a wave packet moves? If there is no fixed coordinate and momenta, then how to see it?

Can at all there be a wave packet? We can't imagine it, since typical wave packet has a fixed momenta, which can't be.
(??? right?)

Can we change uncertainty to the momenta or to coordinate?

(discuss this question about a particle, that how many operators correspond to it? why in the QFT we solve for only one plane wave for the electron? the reason is (maybe!!???) that we can go to the momenta representation and if we don't know anything about coordinate, then it will 100% be fine. is it a good argument?????????????? think about it!!!!)

4.1.3 Concept of Coherent States

(скоро разберусь, пока не вижу еще)

Concept

(it is written in many books, by the way)

Applications of coherent states

(it is written in many books, by the way)

4.1.4 Feynman-Hellmann Theorem

(пока не отработал, нужно доделывать!)

Суть теоремы Фейнмана-Хеллмана

Известно, что среднее значение

$$\frac{\partial f_n}{\partial \lambda} = \left\langle n \left| \frac{\partial \hat{f}}{\partial \lambda} \right| n \right\rangle, \quad \hat{f}|n\rangle = f_n|n\rangle$$

$$\frac{\partial f_n}{\partial \lambda} = \frac{\partial}{\partial \lambda}\langle n|\hat{f}|n\rangle = \left\langle n \left| \frac{\partial \hat{f}}{\partial \lambda} \right| n \right\rangle + \left(\frac{\partial}{\partial \lambda}\langle n|\right)\hat{f}|n\rangle + \left\langle n \left| \hat{f}\left(\frac{\partial}{\partial \lambda}|n\rangle\right)\right.\right.$$

$$\frac{\partial f_n}{\partial \lambda} = \left\langle n \left| \frac{\partial \hat{f}}{\partial \lambda} \right| n \right\rangle + f_n\left(\frac{\partial}{\partial \lambda}\langle n|\right)|n\rangle + f_n\left\langle n \left| \left(\frac{\partial}{\partial \lambda}|n\rangle\right)\right.\right. = \left\langle n \left| \frac{\partial \hat{f}}{\partial \lambda} \right| n \right\rangle + f_n\frac{\partial}{\partial \lambda}\langle n|n\rangle$$

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\Delta + V(\boldsymbol{r})$$

$$\frac{\partial E_n}{\partial \lambda} = 0$$

$$\frac{\partial E_n}{\partial \lambda} = \left\langle n \left| \frac{\partial \hat{H}}{\partial \lambda} \right| n \right\rangle \Bigg|_{\lambda=1}$$

$$\left.\frac{\partial \hat{H}}{\partial \lambda}\right|_{\lambda=1} = 2\frac{\hbar^2}{2m}\frac{1}{\lambda^3}\Delta' + \left.\frac{\partial V(\lambda \boldsymbol{r})}{\partial \lambda \boldsymbol{r}'}\frac{\partial \lambda \boldsymbol{r}'}{\partial \lambda}\right|_{\lambda=1} = -2\hat{T} + \boldsymbol{r}\frac{\partial V(\boldsymbol{r})}{\partial \boldsymbol{r}}$$

$$\left.\frac{\partial \hat{H}}{\partial \lambda}\right|_{\lambda=1} = 2\frac{\hbar^2}{2m}\frac{1}{\lambda^3}\Delta' + \left.\frac{\partial V(\lambda \boldsymbol{r})}{\partial \lambda \boldsymbol{r}'}\frac{\partial \lambda \boldsymbol{r}'}{\partial \lambda}\right|_{\lambda=1} = -2\hat{T} + \boldsymbol{r}\frac{\partial V(\boldsymbol{r})}{\partial \boldsymbol{r}}$$

О применениях соотношения Фейнмана-Хеллмана

(потом напишу, пока не очень применял)

Сила действующая на стенку, пользуясь теоремой Ф-Х (???)

(потом напишу)

Как догадаться про это?

4.1.5 Virial Theorem in QM

(нужно будет - пропишу тут)

4.1.6 Ehrenfest Theorem

(???)

мотивация и обзор

Теорема Эренфеста в двух словах

Важно понимать, что квантование происходит так, что в среднем квантовая система за счет канонического квантования ведет себя так, как классическая.

(что такое "в среднем"??? тут подробно объяснять это нужно)

Это же отражает теорема Эрнфеста. На языке формул в формализме Гамильтона можно записать:

$$\frac{d\langle \hat{q} \rangle}{dt} = \left\langle \frac{\partial H}{\partial p} \right\rangle, \quad \frac{d\langle \hat{p} \rangle}{dt} = -\left\langle \frac{\partial H}{\partial q} \right\rangle$$

$$\mathrm{i}\hbar \frac{d\langle \hat{q} \rangle}{dt} = \langle [\hat{q}, \hat{H}] \rangle = \mathrm{i}\hbar \langle \{q, H\}_{\mathrm{P}} \rangle = \mathrm{i}\hbar \left\langle \frac{\partial H}{\partial p} \right\rangle$$

$$\mathrm{i}\hbar \frac{d\langle \hat{p} \rangle}{dt} = \langle [\hat{p}, \hat{H}] \rangle = \mathrm{i}\hbar \langle \{p, H\}_{\mathrm{P}} \rangle = -\mathrm{i}\hbar \left\langle \frac{\partial H}{\partial q} \right\rangle$$

(суть? применения?)

О применениях теоремы Эрнфеста

(укажу, когда она нужна, пока что не пользовался ни разу и не до неё)
(укажу связи с другими местами, где она используется)

Другое о квантовании

Пространственное квантование (???????????)

(зависла теория общефиза, потом посмотрю.)
Энергия физической системы в зависимости от формы потенциальной кривой может иметь либо непрерывный, либо дискретный спектр.

Как догадаться про это?

4.1.7 Variational Principle

(метод пробных функций для атома гелия тоже тут)

Теория

Если бы действие для динамики волновой функции существовало и имело вид

$$S = \int d^3 r dt \Psi^\dagger(\boldsymbol{r}, t) \left\{ \mathrm{i}\hbar \frac{\partial}{\partial t} - \hat{H} \right\} \Psi(\boldsymbol{r}, t)$$

То с помощью вариации можно было бы получить уравнение Шредингера.
Считая $\Psi, \Psi^\dagger$ независимыми, запишем уравнение Эйлера-Лагранжа:

$$\frac{\delta S}{\delta \Psi^\dagger} = 0 \leftrightarrow \frac{\partial \mathcal{L}}{\partial \Psi^\dagger} = 0 \to \mathrm{i}\hbar \frac{\partial}{\partial t} \Psi - \hat{H}\Psi = 0$$
$$\frac{\delta S}{\delta \Psi} = 0 \leftrightarrow \frac{\partial \mathcal{L}}{\partial \Psi} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \dot{\Psi}} = 0 \to -\Psi^\dagger \hat{H} - \mathrm{i}\hbar \frac{\partial}{\partial t} \Psi^\dagger = 0$$

Другое о вариационном принципе

Почему не очевиден вариационный принцип (??)

(оставшийся вопрос)

О случаях применения вариационного принципа (???)

Заготовки для применения вариационного принципа

Мы только что нашли принцип, из которого можно вывести уравнение Шредингера, посмотрим, что же еще можно из него вывести?
(вроде бы в атоме гелия про него есть примеры)

приближенные оценки энергии стационарных состояний

Вариационный принцип полезен для нахождения энергии стационарных состояний в классе пробных функций.
(алгоритм такой-то)
Покажем на примере, как это происходит:

$$\Psi(q) \simeq e^{-\frac{q^2}{2\sigma^2}}$$

$$\hat{H}\Psi(q) = -\frac{\hbar^2}{2m}\Psi''(q) + \frac{m\omega^2 q^2}{2}\Psi(q)$$

$$N = \int\limits_{-\infty}^{\infty} dq|\Psi(q)|^2 = \int\limits_{-\infty}^{\infty} dq e^{-\frac{q^2}{\sigma^2}} = \left\{ \int\limits_{-\infty}^{\infty} dq dq' e^{-\frac{q^2+q'^2}{\sigma^2}} \right\}^{1/2}$$

$$N = \left\{ \int\limits_{0}^{2\pi} d\varphi \int\limits_{0}^{\infty} r dr e^{-\frac{r^2}{\sigma^2}} \right\}^{1/2} = \sqrt{\pi\sigma^2}$$

$$S_{\text{stat.}} = \frac{1}{\sigma\sqrt{\pi}} \int\limits_{\text{infty}}^{\infty} dq \cdot e^{-\frac{q^2}{\sigma^2}} \left\{ E - \frac{\hbar^2}{2m\sigma^2} - \frac{q^2}{2}\left[m\omega^2 - \frac{\hbar^2}{m\sigma^4} \right] \right\} = E - \frac{\hbar^2}{2m\sigma^2} - \frac{\sigma^2}{4}\left[m\omega^2 - \frac{\hbar^2}{m\sigma^4} \right]$$

$$S'_{\text{stat.}} = \frac{\hbar^2}{4m\sigma^4} - \frac{m\omega^2}{4} = 0, \quad \rightarrow \quad \sigma^2 = \frac{\hbar}{m\omega}$$

$$H = \tfrac{1}{2}\hbar\omega$$
$$S''_{\text{stat.}} = -\tfrac{\hbar^2}{2m\sigma^6} < 0$$

Как догадаться про это?

(????)

4.2 Special Mathematical Transformations and Their Consequences

4.2.1 3. Weyl Relations 1

Let R be an irreducible unitary representation of the Heisenberg group $\mathbf{H}_n$ in Hilbert space $\mathscr{H}$. It follows from Schur's lemma that $R\left(e^{\alpha c}\right) = e^{i\hbar\alpha} I$ for some $\hbar \in \mathbb{R}$, where I is the identity operator on $\mathscr{H}$. If $\hbar = 0$, the n-parameter abelian groups of unitary operators $U(\boldsymbol{u}) = R\left(e^{\boldsymbol{u}X}\right)$ and $V(\boldsymbol{v}) = R\left(e^{\boldsymbol{v}\boldsymbol{Y}}\right)$ commute, so using Schur's lemma once again we conclude that there exist $\boldsymbol{p}, \boldsymbol{q} \in \mathbb{R}^n$ such that $U(\boldsymbol{u}) = e^{-i\boldsymbol{u}\boldsymbol{p}} I$ and $V(\boldsymbol{v}) = e^{-i\boldsymbol{v}\boldsymbol{q}} I$. Therefore, in this case the irreducible representation R is one-dimensional and is parametrized by a vector $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{R}^{2n}$. When $\hbar \neq 0$, unitary operators $U(\boldsymbol{u})$ and $V(\boldsymbol{v})$ satisfy the Weyl relations

$$U(\boldsymbol{u})V(\boldsymbol{v}) = e^{i\hbar\boldsymbol{u}\boldsymbol{v}} V(\boldsymbol{v})U(\boldsymbol{u}) \tag{3.1}$$

which admit the Schrodinger representation, introduced in Section 2.2. It turns out that every unitary irreducible representation of the Heisenberg group $\mathbf{H}_n$ is unitarily equivalent either to a one-dimensional representation with parameters $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{R}^{2n}$, or to the Schrodinger representation with some $\hbar \neq 0$. The physically meaningful case corresponds to $\hbar > 0$, and representation with $-\hbar$ is given by the operators $U^{-1}(\boldsymbol{u}) = U(-\boldsymbol{u})$ and $V(\boldsymbol{v})$.

3.1. Stone-von Neumann theorem.

Here we prove the following fundamental result.

Theorem 3.1 (Stone-von Neumann theorem). Every irreducible unitary representation of the Weyl relations for n degrees of freedom,

$$U(\boldsymbol{u})V(\boldsymbol{v}) = e^{i\hbar \boldsymbol{u}\boldsymbol{v}}V(\boldsymbol{v})U(\boldsymbol{u})$$

is unitarily equivalent to the Schrodinger representation.

Proof. It is sufficient to consider $n = 1$, the general case $n > 1$ is treated similarly. Set

$$S(u, v) = e^{-\frac{i\hbar uv}{2}}U(u)V(v)$$

The unitary operator $S(u, v)$ satisfies

$$S(u, v)^* = S(-u, -v) \tag{3.2}$$

and it follows from the Weyl relation that

$$S(u_1, v_1)\, S(u_2, v_2) = e^{\frac{i\hbar}{2}(u_1v_2 - u_2v_1)} S(u_1 + u_2, v_1 + v_2) \tag{3.3}$$

Define a linear map $W : L^1(\mathbb{R}^2) \to \mathscr{L}(\mathscr{H})$, called the Weyl transform, by

$$W(f) = \frac{1}{2\pi}\int_{\mathbb{R}^2} f(u, v)S(u, v)dudv$$

Here the integral is understood in the weak sense: for every $\psi_1, \psi_2 \in \mathscr{H}$,

$$(W(f)\psi_1, \psi_2) = \frac{1}{2\pi}\int_{\mathbb{R}^2} f(u, v)\,(S(u, v)\psi_1, \psi_2)\, dudv$$

The integral is absolutely convergent for all $\psi_1, \psi_2 \in \mathscr{H}$, and defines a bounded operator $W(f)$ satisfying

$$\|W(f)\| \leq \frac{1}{2\pi}\|f\|_{L^1}$$

The Weyl transform has the following properties.

WT1. For $f \in L^1(\mathbb{R}^2)$,

$$W(f)^* = W(f^*)$$

where

$$f^*(u, v) = \overline{f(-u, -v)}$$

WT2. For $f \in L^1(\mathbb{R}^2)$,

$$S(u_1, v_1)\, W(f) S(u_2, v_2) = W(\tilde{f})$$

where

$$\tilde{f}(u, v) = e^{\frac{i\hbar}{2}\{(u_1-u_2)v-(v_1-v_2)u+u_1v_2-u_2v_1\}} f(u - u_1 - u_2, v - v_1 - v_2)\,.$$

WT3. $\operatorname{Ker} W = \{0\}$

WT4. For $f_1, f_2 \in L^1(\mathbb{R}^2)$,

$$W(f_1)\, W(f_2) = W(f_1 *_\hbar f_2)\,,$$

where

$$(f_1 *_\hbar f_2)(u,v) = \frac{1}{2\pi}\int_{\mathbb{R}^2} e^{\frac{i\hbar}{2}(uv'-u'v)} f_1(u-u', v-v')\, f_2(u',v')\, du'dv'.$$

The first two properties follow from the definition and (3.2) and (3.3). To prove WT3, suppose that $W(f)=0$. Then for every $\psi_1, \psi_2 \in \mathscr{H}$ and all $u', v' \in \mathbb{R}$ we have

$$\begin{aligned} 0 &= (W(f) S(u',v')\,\psi_1, S(u',v')\,\psi_2) \\ &= \frac{1}{2\pi}\int_{\mathbb{R}^2} e^{i\hbar(uv'-u'v)} f(u,v)\,(S(u,v)\psi_1, \psi_2)\, dudv. \end{aligned}$$

Therefore $f(u,v)\,(S(u,v)\psi_1,\psi_2)=0$ a.e. on $\mathbb{R}^2$, so that $f=0$.
To prove WT4, we compute

$$\begin{aligned} (W(f_1)W(f_2)\psi_1,\psi_2) &= (W(f_2)\psi_1, W(f_1)^*\psi_2) \\ &= \frac{1}{2\pi}\int_{\mathbb{R}^2} f_2(u_2,v_2)\,(S(u_2,v_2)\psi_1, W(f_1)^*\psi_2)\, du_2dv_2 \\ &= \frac{1}{2\pi}\int_{\mathbb{R}^2} f_2(u_2,v_2)\,(W(f_1)S(u_2,v_2)\psi_1, \psi_2)\, du_2dv_2 \\ &= \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} f_1(u_1-u_2, v_1-v_2)\, f_2(u_2,v_2)\,. \\ &\quad \cdot e^{\frac{i\hbar}{2}(u_1v_2-u_2v_1)}\,(S(u_1,v_1)\psi_1,\psi_2)\, du_1dv_1du_2dv_2 \\ &= \frac{1}{2\pi}\int_{\mathbb{R}^2} (f_1 *_\hbar f_2)(u,v)\,(S(u,v)\psi_1,\psi_2)\, dudv. \end{aligned}$$

We have $f_1 *_\hbar f_2 \in L^1(\mathbb{R}^2)$, and it follows from the associativity of the operator product and property WT3 that the linear mapping

$$*_\hbar : L^1(\mathbb{R}^2) \times L^1(\mathbb{R}^2) \to L^1(\mathbb{R}^2)$$

defines a new associative product on $L^1(\mathbb{R}^2)$,

$$f_1 *_\hbar (f_2 *_\hbar f_3) = (f_1 *_\hbar f_2) *_\hbar f_3 \text{ for all } f_1, f_2, f_3 \in L^1(\mathbb{R}^2).$$

When $\hbar = 0$, the product $*_\hbar$ becomes the usual convolution product on $L^1(\mathbb{R}^2)$.

For every non-zero $\psi \in \mathscr{H}$ denote by $\mathscr{H}_\psi$ the closed subspace of $\mathscr{H}$ spanned by the vectors $S(u,v)\psi$ for all $u, v \in \mathbb{R}$. The subspace $\mathscr{H}_\psi$ is invariant for all operators $U(u)$ and $V(v)$. Since the representation of the Weyl relation is irreducible, $\mathscr{H}_\psi = \mathscr{H}$.

There is a vector $\psi_0 \in \mathscr{H}$ for which all inner products of the generating vectors $S(u,v)\psi_0$ of $\mathscr{H}_{\psi_0}$ can be explicitly computed. Namely, let

$$f_0(u,v) = \hbar e^{-\frac{\hbar}{4}(u^2+v^2)}$$

and set

$$W_0 = W(f_0)$$

Then $W_0^* = W_0$ and

$$W_0 S(u,v) W_0 = e^{-\frac{\hbar}{4}(u^2+v^2)} W_0.$$

In particular, $W_0^2 = W_0$, so that W_0 is an orthogonal projection. Indeed, using WT4, we have

$$W_0 S(u,v) W_0 = W\left(f_0 *_\hbar \tilde{f}_0\right)$$

where

$$\tilde{f}_0(u',v') = e^{\frac{i\hbar}{2}(uv'-u'v)} f_0(u'-u, v'-v)$$

By "completing the square" we obtain

$$\left(f_0 * \hbar\tilde{f}_0\right)(u',v') = \hbar e^{-\frac{\hbar}{4}\left(u^2+v^2+u'^2+v'^2\right)} I(u',v')$$

where

$$I(u',v') = \frac{\hbar}{2\pi}\int_{\mathbb{R}^2} e^{-\frac{\hbar}{2}\left\{(u''-u-u'+iv+iv')^2+(v''-v-v'-iu-iu')^2\right\}} du''dv''$$

Shifting contours of integration to $\operatorname{Im} u'' = -v-v', \operatorname{Im} v'' = u+u'$ and substituting $\xi = u''-u-u'+iv+iv', \eta = v''-v-v'-iu-iu'$, we get

$$I(u',v') = \frac{\hbar}{2\pi}\int_{\mathbb{R}^2} e^{-\frac{\hbar}{2}\left(\xi^2+\eta^2\right)} d\xi d\eta = 1$$

Now let $\mathscr{H}_0 = \operatorname{Im} W_0$ - a non-zero closed subspace of $\mathscr{H}$ by property WT3.
For every $\psi_1, \psi_2 \in \mathscr{H}_0$ we have $W_0\psi_1 = \psi_1, W_0\psi_2 = \psi_2$, and

$$\begin{aligned}
\left(S(u_1,v_1)\psi_1, S(u_2,v_2)\psi_2\right) &= \left(S(u_1,v_1) W_0\psi_1, S(u_2,v_2) W_0\psi_2\right) \\
&= \left(W_0 S(-u_2,-v_2) S(u_1,v_1) W_0\psi_1, \psi_2\right) \\
&= e^{\frac{i\hbar}{2}(u_1v_2-u_2v_1)}\left(W_0 S(u_1-u_2, v_1-v_2) W_0\psi_1, \psi_2\right) \\
&= e^{\frac{i\hbar}{2}(u_1v_2-u_2v_1)-\frac{\hbar}{4}\left\{(u_1-u_2)^2+(v_1-v_2)^2\right\}}\left(W_0\psi_1, \psi_2\right) \\
&= e^{\frac{i\hbar}{2}(u_1v_2-u_2v_1)-\frac{\hbar}{4}\left\{(u_1-u_2)^2+(v_1-v_2)^2\right\}}\left(\psi_1, \psi_2\right)
\end{aligned}$$

This implies that the subspace $\mathscr{H}_0$ is one-dimensional. Indeed, for every $\psi_1, \psi_2 \in \mathscr{H}_0$ such that $(\psi_1, \psi_2) = 0$, we have that the corresponding subspaces $\mathscr{H}_{\psi_1}$ and $\mathscr{H}_{\psi_2}$ are orthogonal. Since $\mathscr{H}_\psi = \mathscr{H}$ for every non-zero ψ, at least one of the vectors ψ_1, ψ_2 is 0 . Let $\mathscr{H}_0 = \mathbb{C}\psi_0, \|\psi_0\| = 1$, and set

$$\psi_{\alpha,\beta} = S(\alpha,\beta)\psi_0, \quad \alpha,\beta \in \mathbb{R}.$$

The closure of the linear span of the vectors $\psi_{\alpha,\beta}$ for all $\alpha,\beta \in \mathbb{R}$ is $\mathscr{H}$. We have

$$\left(\psi_{\alpha,\beta}, \psi_{\gamma,\delta}\right) = e^{\frac{i\hbar}{2}(\alpha\delta-\beta\gamma)-\frac{\hbar}{4}\left\{(\alpha-\gamma)^2+(\beta-\delta)^2\right\}}$$

and

$$S(u,v)\psi_{\alpha,\beta} = e^{\frac{i\hbar}{2}(u\beta-v\alpha)}\psi_{\alpha+u,\beta+v}.$$

Next we consider the Schrodinger representation of the Weyl relation in $L^2(\mathbb{R}, dq)$:

$$\begin{aligned}
(\mathrm{U}(u)\varphi)(q) &= \varphi(q-\hbar u) \\
(\mathrm{V}(v)\varphi)(q) &= e^{-ivq}\varphi(q) \\
(\mathrm{S}(u,v)\varphi)(q) &= e^{\frac{i\hbar}{2}uv-ivq}\varphi(q-\hbar u)
\end{aligned}$$

For the corresponding operator W_0 we have

$$
\begin{aligned}
\left(\mathbf{W}_0\varphi\right)(q) &= \frac{\hbar}{2\pi}\int_{\mathbb{R}^2} e^{-\frac{\hbar}{4}\left(u^2+v^2\right)} e^{\frac{i\hbar}{2}uv-ivq}\varphi(q-\hbar u)dudv \\
&= \sqrt{\frac{\hbar}{\pi}}\int_{-\infty}^{\infty} e^{-\frac{\hbar}{4}\left\{u^2+\left(u-\frac{2}{\hbar}q\right)^2\right\}}\varphi(q-\hbar u)du \\
&= \frac{1}{\sqrt{\hbar\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2\hbar}\left(q^2+q'^2\right)}\varphi\left(q'\right)dq',
\end{aligned}
$$

so that W_0 is a projection onto the one-dimensional subspace of $L^2(\mathbb{R},dq)$ spanned by the Gaussian exponential $\varphi_0(q)=\frac{1}{\sqrt[4]{\pi\hbar}}e^{-\frac{1}{2\hbar}q^2}$, $\|\varphi_0\|=1$. Let

$$\varphi_{\alpha,\beta}=\mathrm{S}(\alpha,\beta)\varphi_0.$$

Since the Schrodinger representation is irreducible, the closed subspace spanned by the functions $\varphi_{\alpha,\beta}$ for all $\alpha,\beta\in\mathbb{R}$ is the whole Hilbert space $L^2(\mathbb{R},dq)$. (This also follows from the completeness of Hermite-Tchebyscheff functions, since $\varphi_{\alpha,\beta}(q)=\frac{1}{\sqrt[4]{\pi\hbar}}e^{\frac{i\hbar}{2}\alpha\beta-i\beta q-\frac{1}{2\hbar}(q-\hbar\alpha)^2}$.) We have

$$\left(\varphi_{\alpha,\beta},\varphi_{\gamma,\delta}\right)=e^{\frac{i\hbar}{2}(\alpha\delta-\beta\gamma)-\frac{\hbar}{4}\left\{(\alpha-\gamma)^2+(\beta-\delta)^2\right\}}$$

and

$$\mathrm{S}(u,v)\varphi_{\alpha,\beta}=e^{\frac{i\hbar}{2}(u\beta-v\alpha)}\varphi_{\alpha+u,\beta+v}.$$

For $\psi=\sum_{i=1}^n c_i\psi_{\alpha_i,\beta_i}\in\mathscr{H}$ define

$$\mathscr{U}(\psi)=\sum_{i=1}^n c_i\varphi_{\alpha_i,\beta_i}\in L^2(\mathbb{R},dq)$$

Since inner products between the vectors $\psi_{\boldsymbol{\alpha},\beta}$ coincide with the inner products between the vectors $\varphi_{\alpha,\beta}$, we have

$$\|\mathscr{U}(\psi)\|_{L^2}^2=\|\psi\|_{\mathscr{H}}^2,$$

so that $\mathscr{U}$ is a well-defined unitary operator between the subspaces spanned by the vectors $\{\psi_{\alpha,\beta}\}_{\alpha,\beta\in\mathbb{R}}$ and $\{\varphi_{\alpha,\beta}\}_{\alpha,\beta\in\mathbb{R}}$. Thus $\mathscr{U}$ extends to the unitary operator $\mathscr{U}:\mathscr{H}\to L^2(\mathbb{R},dq)$ and

$$\mathscr{U}\,S(\alpha,\beta)=\mathrm{S}(\alpha,\beta)\mathscr{U}\quad\text{ for all }\quad\alpha,\beta\in\mathbb{R}.$$

Lemma 2.1 in Section 2.1 is now an easy corollary of the Stone-von Neumann theorem.

Corollary 3.2. The self-adjoint generators $\boldsymbol{P}=(P_1,...,P_n)$ and $\boldsymbol{Q}=(Q^1,...,Q^n)$ of the n-parameter abelian groups of unitary operators $U(\boldsymbol{u})$ and $V(\boldsymbol{v})$ satisfy Heisenberg commutation relations.

Proof. It follows from the Stone theorem that in the Schrodinger representation the generators $\boldsymbol{P}$ and $\boldsymbol{Q}$ are momenta and coordinate operators.

Remark. For n degrees of freedom

$$S(\boldsymbol{u},\boldsymbol{v})=e^{-\frac{i\hbar}{2}\boldsymbol{uv}}U(\boldsymbol{u})V(\boldsymbol{v})=e^{-\frac{i\hbar}{2}\boldsymbol{uv}}e^{-i\boldsymbol{uP}}e^{-i\boldsymbol{vQ}}$$

and formally using the Baker-Campbell-Hausdorff formula, we get

$$S(\boldsymbol{u},\boldsymbol{v})=e^{-i(\boldsymbol{uP}+\boldsymbol{vQ})}\tag{3.4}$$

Thus the Weyl transform

$$W(f) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} f(\boldsymbol{u}, \boldsymbol{v}) e^{-i(\boldsymbol{uP}+\boldsymbol{vQ})} d^n\boldsymbol{u} d^n\boldsymbol{v}$$

can be considered as a non-commutative Fourier transform - an operatorvalued generalization of the "ordinary" Fourier transform

$$\hat{f}(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} f(\boldsymbol{u}, \boldsymbol{v}) e^{-i(\boldsymbol{up}+\boldsymbol{vq})} d^n\boldsymbol{u} d^n\boldsymbol{v}$$

Remark. The Stone-von Neumann theorem is a very strong result. In particular, it implies that creation and annihilation operators for n degrees of freedom,

$$\boldsymbol{a} = \frac{1}{\sqrt{2\hbar}}(\boldsymbol{Q} + i\boldsymbol{P}), \quad \boldsymbol{a}^* = \frac{1}{\sqrt{2\hbar}}(\boldsymbol{Q} - i\boldsymbol{P})$$

where $\boldsymbol{P}$ and $\boldsymbol{Q}$ are the corresponding generators [24] satisfying Heisenberg commutation relations, are unitarily equivalent to the corresponding operators in the Schrodinger representation. Thus there always exists a ground state - a vector $\psi_0 \in \mathscr{H}$, annihilated by the operators $\boldsymbol{a} = (a_1, ..., a_n)$. The corresponding statement no longer holds for quantum systems with infinitely many degrees of freedom, described by quantum field theory, where one needs to postulate the existence of the ground state (the "physical vacuum").

The Weyl transform in the Schrodinger representation $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ can be described explicitly as a bounded operator with an integral kernel. Namely,

$$(S(\boldsymbol{u}, \boldsymbol{v})\psi)(\boldsymbol{q}) = e^{\frac{i\hbar}{2}\boldsymbol{uv} - i\boldsymbol{vq}} \psi(\boldsymbol{q} - \hbar\boldsymbol{u}), \quad \psi \in L^2(\mathbb{R}^n, d^n\boldsymbol{q}) \tag{3.5}$$

and for $\psi_1, \psi_2 \in L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ and $f \in L^1(\mathbb{R}^{2n}) \cap L^2(\mathbb{R}^{2n})$ we have

$$\begin{aligned}(W(f)\psi_1, \psi_2) &= \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} f(\boldsymbol{u}, \boldsymbol{v}) \left(S(\boldsymbol{u}, \boldsymbol{v})\psi_1, \psi_2\right) d^n\boldsymbol{u} d^n\boldsymbol{v} \\ = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} &\left(\int_{\mathbb{R}^n} e^{\frac{i\hbar}{2}\boldsymbol{uv} - i\boldsymbol{vq}} f(\boldsymbol{u}, \boldsymbol{v}) \psi_1(\boldsymbol{q} - \hbar\boldsymbol{u}) \overline{\psi_2(\boldsymbol{q})} d^n\boldsymbol{q} \right) d^n\boldsymbol{u} d^n\boldsymbol{v} \\ &= \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} K(\boldsymbol{q}, \boldsymbol{q}') \psi_1(\boldsymbol{q}') d^n\boldsymbol{q}' \right) \overline{\psi_2(\boldsymbol{q})} d^n\boldsymbol{q}\end{aligned}$$

where

$$K(\boldsymbol{q}, \boldsymbol{q}') = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} f\left(\frac{\boldsymbol{q} - \boldsymbol{q}'}{\hbar}, \boldsymbol{v}\right) e^{-\frac{i}{2}(\boldsymbol{q}+\boldsymbol{q}')\boldsymbol{v}} d^n\boldsymbol{v} \tag{3.6}$$

The interchange of the order of integrations is justified by the Fubini theorem. Thus $W(f)$ is an integral operator with the integral kernel $K(\boldsymbol{q}, \boldsymbol{q}')$,

$$(W(f)\psi)(\boldsymbol{q}) = \int_{\mathbb{R}^n} K(\boldsymbol{q}, \boldsymbol{q}') \psi(\boldsymbol{q}') d^n\boldsymbol{q}', \quad \psi \in L^2(\mathbb{R}^n, d^n\boldsymbol{q}).$$

By the Plancherel theorem,

$$\int_{\mathbb{R}^{2n}} |K(\boldsymbol{q}, \boldsymbol{q}')|^2 d^n\boldsymbol{q} d^n\boldsymbol{q}' = \int_{\mathbb{R}^{2n}} |f(\boldsymbol{u}, \boldsymbol{v})|^2 d^n\boldsymbol{u} d^n\boldsymbol{v}$$

so that $W(f)$ is a Hilbert-Schmidt operator on $\mathscr{H}$. The linear subspace $L^1(\mathbb{R}^{2n}) \cap L^2(\mathbb{R}^{2n})$ is dense in $L^2(\mathbb{R}^{2n})$ and the Weyl transform extends to the isometry $W : L^2(\mathbb{R}^{2n}) \to \mathscr{S}_2$, where $\mathscr{S}_2$ is the Hilbert space of HilbertSchmidt operators on $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$. Since every

Hilbert-Schmidt operator on $\mathscr{H}$ is a bounded operator with the integral kernel in $L^2(\mathbb{R}^{2n})$, the mapping W is onto. Thus we have proved the following result.

Lemma 3.1. The Weyl transform W defines the isomorphism $L^2(\mathbb{R}^{2n}) \simeq \mathscr{S}_2$.

Problem 3.

1. Let $\boldsymbol{P} = (P_1, ..., P_n)$ and $\boldsymbol{Q} = (Q_1, ..., Q_n)$ be self-adjoint operators [25] on $\mathscr{H}$ satisfying Heisenberg commutation relations (2.4) on some dense domain D in $\mathscr{H}$, and such that the symmetric operator $H = \sum_{k=1}^{n}(P_k^2 + Q_k^2)$, defined on D, is essentially self-adjoint. Also suppose that every bounded operator which commutes with $\boldsymbol{P}$ and $\boldsymbol{Q}$ is a multiple of the identity operator in $\mathscr{H}$. Prove that $\boldsymbol{P}$ and $\boldsymbol{Q}$ are unitarily equivalent to momenta and coordinate operators in the Schrodinger representation. (Hint: By the Stone-von Neumann theorem, it is sufficient to show that $\boldsymbol{P}$ and $\boldsymbol{Q}$ define an integrable representation of the Heisenberg algebra. One can also prove this result directly by using commutation relations between the operators $H, a^*, \boldsymbol{a}$ and the arguments in Section 2.6. This would give another proof of the Stone-von Neumann theorem.)

Problem 3.

2. Prove formula (3.4).

3.2. Invariant formulation.

Here we present a coordinate-free description of the Schrodinger representation. Let (V, ω) be a finite-dimensional symplectic vector space, $\dim V = 2n$. Recall that (see Section 2.1) the Heisenberg algebra $\mathfrak{g} = \mathfrak{g}(V)$ is a one-dimensional central extension of the abelian Lie algebra V by the skew-symmetric bilinear form ω. As a vector space,

$$\mathfrak{g} = V \oplus \mathbb{R}c$$

with the Lie bracket

$$[u + \alpha c, v + \beta c] = \omega(u, v)c, \quad u, v \in V, \quad \alpha, \beta \in \mathbb{R}$$

Every Lagrangian subspace ℓ of V defines an abelian subalgebra $\ell \oplus \mathbb{R}c$ of g. A Lagrangian subspace ℓ' is complementary to ℓ in V if $\ell \oplus \ell' = V$. A choice of the complementary Lagrangian subspace ℓ' to ℓ establishes the isomorphism

$$\mathfrak{g}/(\ell \oplus \mathbb{R}c) \simeq \ell'$$

The Heisenberg group $G = G(V)$ is a connected and simply-connected Lie group with the Lie algebra $\mathfrak{g}$. By the exponential map, $G \simeq V \oplus \mathbb{R}c$ as a manifold, with the group law

$$\exp(v_1 + \alpha_1 c)\exp(v_2 + \alpha_2 c) = \exp\left(v_1 + v_2 + \left(\alpha_1 + \alpha_2 + \frac{1}{2}\omega(v_1, v_2)\right)c\right)$$

where $v_1, v_2 \in V, \alpha_1, \alpha_2 \in \mathbb{R}$. A choice of the symplectic basis for V establishes the isomorphism $G(V) \simeq \mathbf{H}_n$ with the matrix Heisenberg group defined in Section 2.1. The volume form

[024] Here it is convenient to lower the indices by the Euclidean metric on $\mathbb{R}^n$ and use $Q = (Q_1, ..., Q_n)$.

$d^{2n}\boldsymbol{v} \wedge dc$, where $d^{2n}\boldsymbol{v} \in \Lambda^{2n}V^*$ is a volume form on V and V^* is the dual vector space to V, defines a bi-invariant Haar measure on G. Every Lagrangian subspace ℓ defines an

abelian subgroup $L = \exp(\ell \oplus \mathbb{R}c)$ of G, and a choice of the complementary Lagrangian subspace ℓ' establishes the isomorphism

$$G/L \simeq \ell'. \tag{3.7}$$

The isomorphism $\Lambda^{2n}V^* \simeq \Lambda^n\ell^* \wedge \Lambda^n\ell'^*$ gives rise to the volume form $d^n\boldsymbol{v}'$ on ℓ' and defines a measure dg on the homogeneous space G/L. The measure dg is invariant under the left G-action and does not depend on the choice of ℓ'.

For a given $\hbar \in \mathbb{R}$, the function $\chi : L \to \mathbb{C}$,

$$\chi(\exp(v + \alpha c)) = e^{i\hbar\alpha}, \quad v \in V, \alpha \in \mathbb{R},$$

defines a one-dimensional unitary character of L,

$$\chi(l_1 l_2) = \chi(l_1)\chi(l_2), \quad l_1, l_2 \in L.$$

Definition. The Schrodinger representation S_ℓ of the Heisenberg group $G(V)$, associated with a Lagrangian subspace ℓ of V, is a representation of G induced by the one-dimensional representation χ of the corresponding abelian Lie group L,

$$S_\ell = \mathrm{Ind}_L^G \chi.$$

By definition of the induced representation, the Hilbert space $\mathscr{H}_\ell$ of the representation S_ℓ consists of measurable functions $f : G \to \mathbb{C}$ satisfying the property

$$f(gl) = \chi(l)^{-1} f(g), \quad g \in G, l \in L,$$

and such that

$$\|f\|^2 = \int_{G/L} |f(g)|^2 dg < \infty.$$

Corresponding unitary operators $S_\ell(g), g \in G$, are defined by the left translations,

$$(S_\ell(g)f)(g') = f\left(g^{-1}g'\right), \quad f \in \mathscr{H}_\ell, g \in G.$$

In particular,

$$(S_\ell(\exp \alpha c)f)(g) = f(\exp(-\alpha c)g) = f(g\exp(-\alpha c)) = e^{i\hbar\alpha} f(g),$$

so that $S_\ell(\exp \alpha c) = e^{i\hbar\alpha} I$, where I is the identity operator on $\mathscr{H}_\ell$.

For every Lagrangian subspace ℓ of V, the representation S_ℓ is unitarily equivalent to the Schrodinger representation. This can be explicitly shown as follows. By (3.7), a choice of a complementary Lagrangian subspace ℓ' gives rise to the unique decomposition $g = \exp v' \exp(v + \alpha c)$, and for $f \in \mathscr{H}_\ell$ we get

$$f(g) = f(\exp v' \exp(v + \alpha c)) = e^{-i\hbar\alpha} f(\exp v'), \quad v \in \ell, v' \in \ell', \alpha \in \mathbb{R}.$$

Thus every $f \in \mathscr{H}_\ell$ is completely determined by its restriction to $\exp \ell' \simeq \ell'$, and the mapping $\mathscr{U}_\ell : \mathscr{H}_\ell \to L^2(\ell', d^n\boldsymbol{v}')$, defined by

[025] See previous footnote.

$$\mathscr{U}_\ell(f)\,(v') = f\left(\exp\frac{1}{\hbar}v'\right), \quad v' \in \ell',$$

is the isomorphism of Hilbert spaces. For the corresponding representation $\mathrm{S}_\ell = \mathscr{U}_\ell S_\ell \mathscr{U}_\ell^{-1}$ in $L^2\,(\ell', d^n v')$ we have

$$\begin{aligned}(\mathrm{S}_\ell(\exp v)\psi)\,(v') &= e^{i\omega(v,v')}\psi\,(v'), \quad v \in \ell, v' \in \ell' \\ (\mathrm{S}_\ell\,(\exp u')\,\psi)\,(v') &= \psi\,(v' - \hbar u'), \quad u', v' \in \ell'\end{aligned}$$

Let $e^1, ..., e^n, f_1, ..., f_n$ be the symplectic basis for V such that

$$\ell = \mathbb{R}e^1 \oplus \cdots \oplus \mathbb{R}e^n \quad \text{and} \quad \ell' = \mathbb{R}f_1 \oplus \cdots \oplus \mathbb{R}f_n$$

and let $(\boldsymbol{p}, \boldsymbol{q}) = (p_1, ..., p_n, q^1, ..., q^n)$ be the corresponding coordinates in V (see Section 2.6 in Chapter 1). Then $L^2\,(\ell', d^n\boldsymbol{v}') \simeq L^2\,(\mathbb{R}^n, d^n\boldsymbol{q})$ and

$$\mathrm{S}_\ell(\exp \boldsymbol{u}X) = U(\boldsymbol{u}) \quad \text{and} \quad \mathrm{S}_\ell(\exp \boldsymbol{v}Y) = V(\boldsymbol{v})$$

where $\boldsymbol{u}X = \sum_{k=1}^n u^k f_k, \boldsymbol{v}Y = \sum_{k=1}^n v_k e^k$, and $U(\boldsymbol{u}) = e^{-i\boldsymbol{u}\boldsymbol{P}}, V(\boldsymbol{v}) = e^{-i\boldsymbol{v}Q}$ are, respectively, n-parameter groups of unitary operators corresponding to momenta and coordinate operators $\boldsymbol{P}$ and $\boldsymbol{Q}$.

The mapping $*_\hbar$ - the new associative product on $L^1\,(\mathbb{R}^{2n})$ introduced in the last section - can also be described in invariant terms. Let $B_\hbar = G/\Gamma_\hbar$ be the quotient group, where $\Gamma_\hbar = \left\{\exp\left(\frac{2\pi n}{\hbar}c\right) \in G \middle|\ n \in \mathbb{Z}\right\}$ is a discrete central subgroup in G, and let $db = d^{2n}v \wedge d^*\alpha$ be the left-invariant Haar measure on $B_\hbar$, where $d^*\alpha$ is the normalized Haar measure on the circle $\mathbb{R}/\frac{2\pi}{\hbar}\mathbb{Z}$. The Banach space $L^1\,(B_\hbar, db)$ has an algebra structure with respect to the convolution:

$$(\varphi_1 *_{B_\hbar} \varphi_2)\,(b) = \int_{B_\hbar} \varphi_1\,(b_1)\,\varphi_2\left(b_1^{-1}b\right) db_1, \quad \varphi_1, \varphi_2 \in L^1\,(B_\hbar, db)$$

The correspondence

$$L^1\left(V, d^{2n}\boldsymbol{v}\right) \ni f(v) \mapsto \varphi(\exp(v + \alpha c)) = e^{-i\hbar\alpha} f(v) \in L^1\,(B_\hbar, db)$$

defines the inclusion map $L^1\,(V, d^{2n}\boldsymbol{v}) \hookrightarrow L^1\,(B_\hbar, db)$, and the image of $L^1\,(V, d^{2n}\boldsymbol{v})$ is a subalgebra of $L^1\,(B_\hbar, db)$ under the convolution. We have for $f_1, f_2 \in L^1\,(V, d^{2n}v)$,

$$\begin{aligned}(\varphi_1 *_{B_\hbar} \varphi_2)\,(\exp v) &= \int_{B_\hbar} \varphi_1(\exp(u + \alpha c))\varphi_2(\exp(-u - \alpha c)\exp v) d^{2n}\boldsymbol{v} d^*\alpha \\ &= \int_V \varphi_1(\exp u)\varphi_2\left(\exp(v - u)\exp\left(-\frac{1}{2}\omega(u, v)c\right)\right) d^{2n}\boldsymbol{v} \\ &= \int_V f_1(u) f_2(v - u) e^{\frac{i\hbar}{2}\omega(u,v)} d^{2n}\boldsymbol{v} \\ &= (f_1 *_\hbar f_2)\,(v), \quad v \in V\end{aligned}$$

Problem 3.

3. Prove that the Weyl transform is the restriction to $L^1\,(V, d^{2n}\boldsymbol{v})$ of the mapping

$$L^1\,(B_\hbar, db) \ni \varphi \mapsto \int_{B_\hbar} \varphi(b) S_\ell(b) db \in \mathscr{L}\,(\mathscr{H}_\ell)\,.$$

Problem 3.

4. Let ℓ_1, ℓ_2, ℓ_3 be Lagrangian subspaces of V. Define the triple Maslov index $\tau(\ell_1, \ell_2, \ell_3)$ as a signature of the quadratic form Q on $\ell_1 \oplus \ell_2 \oplus \ell_3$, defined by

$$Q(x_1, x_2, x_3) = \omega(x_1, x_2) + \omega(x_2, x_3) + \omega(x_3, x_1).$$

For Lagrangian subspaces ℓ_1, ℓ_2 of V let $\mathscr{F}_{\ell_2,\ell_1}$ be the unitary operator establishing the Hilbert space isomorphism $\mathscr{H}_{\ell_1} \simeq \mathscr{H}_{\ell_2}$ and intertwining representations S_{ℓ_1} and S_{ℓ_2},

$$\mathscr{F}_{\ell_2,\ell_1} S_{\ell_1}(g) = S_{\ell_2}(g) \mathscr{F}_{\ell_2,\ell_1}, \quad g \in G.$$

Prove that $\mathscr{F}_{\ell_1,\ell_3} \mathscr{F}_{\ell_3,\ell_2} \mathscr{F}_{\ell_2,\ell_1} = e^{-\pi i \tau(\ell_1,\ell_2,\ell_3)} I_1$, where I_1 is the identity operator in $\mathscr{H}_{\ell_1}$.

Problem 3.

5. Let $\mathrm{Sp}(V)$ be the symplectic group of (V, ω) - the subgroup of $\mathrm{GL}(V)$, preserving the symplectic form ω. The group $\mathrm{Sp}(V)$ acts as a group of automorphisms of the Heisenberg group G by the formula $h \cdot \exp(v + \alpha c) = \exp(h \cdot v + \alpha c), h \in \mathrm{Sp}(V), v \in V$. Let R be an irreducible unitary representation of G in the Hilbert space $\mathscr{H}$. Show that there exist unitary operators $U(h)$, defined up to multiplication by complex numbers of modulus 1, such that

$$U(h) R(g) U(h)^{-1} = R(h \cdot g), \quad h \in \mathrm{Sp}(V), \quad g \in G,$$

and that U defines a projective unitary representation of $\mathrm{Sp}(V)$ in $\mathscr{H}$, called the Shale-Weil representation. Find a realization of the Hilbert space $\mathscr{H}$ such that the 2-cocycle of the Shale-Weil representation is explicitly computed in terms of the Maslov index.

4.2.2 3. Weyl Relations 2

3.3. Weyl quantization

The Weyl transform, introduced in Section 3.1, defines a quantization of classical systems associated with the phase space $\mathbb{R}^{2n}$ with coordinates $\boldsymbol{p} = (p_1, ..., p_n), \boldsymbol{q} = (q^1, ..., q^n)$, and the Poisson bracket $\{,\} associated with the canonical symplectic form \omega = d\boldsymbol{p} \wedge d\boldsymbol{q}$. Let

$$\Phi = W \circ \mathscr{F}^{-1} : \mathscr{S}\left(\mathbb{R}^{2n}\right) \to \mathscr{L}(\mathscr{H})$$

where W is the Weyl transform and $\mathscr{F}^{-1}$ is the inverse Fourier transform, be the linear mapping of the Schwartz space $\mathscr{S}(\mathbb{R}^{2n})$ of complex-valued functions of rapid decay on $\mathbb{R}^{2n}$ into the Banach space of bounded operators $\mathscr{L}(\mathscr{H})$ on $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$. It is given explicitly by the integral

$$\Phi(f) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} \check{f}(\boldsymbol{u}, \boldsymbol{v}) S(\boldsymbol{u}, \boldsymbol{v}) d^n\boldsymbol{u} d^n\boldsymbol{v}$$

understood as a limit of Riemann sums in the uniform topology on $\mathscr{L}(\mathscr{H})$, where

$$\check{f}(\boldsymbol{u}, \boldsymbol{v}) = \mathscr{F}^{-1}(f)(\boldsymbol{u}, \boldsymbol{v}) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} f(\boldsymbol{p}, \boldsymbol{q}) e^{i(\boldsymbol{up}+\boldsymbol{vq})} d^n\boldsymbol{p} d^n\boldsymbol{q}$$

and $S(\boldsymbol{u}, \boldsymbol{v}) = e^{-\frac{i\hbar}{2}\boldsymbol{uv}} U(\boldsymbol{u}) V(\boldsymbol{v})$. It follows from (3.6) that $\Phi(f)$ is an integral operator: for every $\psi \in L^2(\mathbb{R}^n, d^n\boldsymbol{q})$,

$$(\Phi(f)\psi)(\boldsymbol{q}) = \int_{\mathbb{R}^n} K(\boldsymbol{q},\boldsymbol{q}')\,\psi(\boldsymbol{q}')\,d^n\boldsymbol{q}'$$

where

$$\begin{aligned} K(\boldsymbol{q},\boldsymbol{q}') &= \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} \check{f}\left(\frac{\boldsymbol{q}-\boldsymbol{q}'}{\hbar},\boldsymbol{v}\right) e^{-\frac{i}{2}\boldsymbol{v}(\boldsymbol{q}+\boldsymbol{q}')} d^n\boldsymbol{v} \\ &= \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} f\left(\boldsymbol{p},\frac{\boldsymbol{q}+\boldsymbol{q}'}{2}\right) e^{\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{q}-\boldsymbol{q}')} d^n\boldsymbol{p} \end{aligned}$$

Since the Schwartz space is self-dual with respect to the Fourier transform, $K \in \mathscr{S}(\mathbb{R}^n\times\mathbb{R}^n) \subset L^2(\mathbb{R}^n\times\mathbb{R}^n)$, so that $\Phi(f)$ is a Hilbert-Schmidt operator. Using the property $S(\boldsymbol{u},\boldsymbol{v})^* = S(-\boldsymbol{u},-\boldsymbol{v})$ we get

$$\Phi(f)^* = \Phi(\bar{f})$$

so that classical observables - real-valued functions on $\mathbb{R}^{2n}$, correspond to quantum observables - self-adjoint operators in $\mathscr{H}$. It follows from the property WT3 in Section 3.1 that the mapping Φ is injective; its image $\operatorname{Im}\Phi$ and the inverse mapping Φ^{-1} are explicitly described as follows.

Proposition 3.1. The subspace $\operatorname{Im}\Phi \subset \mathscr{L}(\mathscr{H})$ consists of operators $B \in \mathscr{S}_1$ such that corresponding functions $g(\boldsymbol{u},\boldsymbol{v}) = \hbar^n \operatorname{Tr}(BS(\boldsymbol{u},\boldsymbol{v})^{-1})$ belong to the Schwartz class $\mathscr{S}(\mathbb{R}^{2n})$; in this case $W(g) = B$. The inverse mapping $\Phi^{-1} = \mathscr{F}\circ W^{-1}$ is given by the Weyl's inversion formula

$$\check{f}(\boldsymbol{u},\boldsymbol{v}) = \hbar^n \operatorname{Tr}\left(\Phi(f)S(\boldsymbol{u},\boldsymbol{v})^{-1}\right), \quad f \in \mathscr{S}\left(\mathbb{R}^{2n}\right)$$

Proof. First consider the case $n = 1$. Let

$$H = \frac{P^2+Q^2}{2}$$

be the Hamiltonian of the harmonic oscillator with $m = 1$ and $\omega = 1$. According to Theorem 2.1, the operator H has a complete orthonormal system of real-valued eigenfunctions $\psi_n(q)$, given by Hermite-Tchebyscheff functions, with the eigenvalues $\hbar\left(n+\frac{1}{2}\right)$, so that the inverse operator $H^{-1} \in \mathscr{S}_2$. The operator $H\Phi(f)$ is an integral operator with the kernel $\frac{1}{2}\left(-\hbar^2\frac{\partial^2}{\partial q^2} + q^2\right)K(q,q')$, which is a Schwartz class function on $\mathbb{R}^2$, so that $H\Phi(f) \in \mathscr{S}_2$. The operator

$$\Phi(f) = H^{-1}H\Phi(f)$$

is a product of Hilbert-Schmidt operators and, therefore, is of trace class. Using the orthonormal basis $\{\psi_n(q)\}_{n=0}^{\infty}$ for $\mathscr{H} = L^2(\mathbb{R})$, we get

$$K(q,q') = \sum_{m,n=0}^{\infty} c_{mn}\psi_n(q)\psi_m(q') \tag{3.8}$$

where

$$c_{mn} = \int_{\mathbb{R}^2} K(q,q')\,\psi_n(q)\psi_m(q')\,dqdq'$$

and the series (3.8) converges in $L^2(\mathbb{R}^2)$. Since $K \in \mathscr{S}(\mathbb{R}^2)$, it follows from the N-representation theorem (see Problem 2.13) that this series is also convergent in the $\mathscr{S}(\mathbb{R}^2)$ topology. It is this fact which allows us to set $q' = q$ in (3.8) and to get the expansion

$$K(q,q)=\sum_{m,n=0}^{\infty}c_{mn}\psi_n(q)\psi_m(q)$$

which converges in $\mathscr{S}(\mathbb{R})$. Thus we obtain

$$\operatorname{Tr}\Phi(f)=\sum_{n=0}^{\infty}(\Phi(f)\psi_n,\psi_n)=\sum_{n=0}^{\infty}c_{nn}=\int_{-\infty}^{\infty}K(q,q)dq$$

where the interchange of orders of summation and integration is legitimate.
The general case $n>1$ is similar. We consider the operator

$$H=\frac{\boldsymbol{P}^2+\boldsymbol{Q}^2}{2}$$

and use the fact that operators $H^n\Phi(f)$ and H^{-n} are Hilbert-Schmidt. To prove the formula

$$\operatorname{Tr}\Phi(f)=\int_{\mathbb{R}^n}K(\boldsymbol{q},\boldsymbol{q})d^n\boldsymbol{q}$$

we expand the kernel $K(\boldsymbol{q},\boldsymbol{q}')$ using the orthonormal basis $\{\psi_{\boldsymbol{k}}(\boldsymbol{q})\}_{\boldsymbol{k},=0}^{\infty}$ for $L^2(\mathbb{R}^n)$, where

$$\psi_{\boldsymbol{k}}(\boldsymbol{q})=\psi_{k_1}(q_1)\cdots\psi_{k_n}(q_n),\quad \boldsymbol{k}=(k_1,...,k_n)$$

From the explicit form of the kernel K we get

$$\operatorname{Tr}\Phi(f)=\frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\check{f}(0,\boldsymbol{v})e^{-i\boldsymbol{vq}}d^n\boldsymbol{v}d^n\boldsymbol{q}=\hbar^{-n}\check{f}(0,0)\tag{3.9}$$

which gives the inversion formula for $\boldsymbol{u}=\boldsymbol{v}=0$. To get the inversion formula for all $\boldsymbol{u},\boldsymbol{v}\in\mathbb{R}^n$, it is sufficient to apply (3.9) to the function $f_{uv}=\mathscr{F}\left(\check{f}_{u,v}\right)$, where

$$\check{f}_{\boldsymbol{u},\boldsymbol{v}}(\boldsymbol{u}',\boldsymbol{v}')=\check{f}(\boldsymbol{u}+\boldsymbol{u}',\boldsymbol{v}+\boldsymbol{v}')\,e^{\frac{i\hbar}{2}(\boldsymbol{v}'\boldsymbol{u}-\boldsymbol{u}'\boldsymbol{v})}$$

and to use $S(\boldsymbol{u},\boldsymbol{v})^{-1}=S(\boldsymbol{u},\boldsymbol{v})^*=S(-\boldsymbol{u},-\boldsymbol{v})$ and the property WT2 in Section 3.1,

$$W(\check{f})S(-\boldsymbol{u},-\boldsymbol{v})=W\left(\check{f}_{\boldsymbol{u},\boldsymbol{v}}\right)$$

To complete the proof, we need to show that $\operatorname{Im}\Phi$ consists of all $B\in\mathscr{S}_1$ with the property that the function $g(\boldsymbol{u},\boldsymbol{v})=\hbar^n\operatorname{Tr}\left(BS(\boldsymbol{u},\boldsymbol{v})^{-1}\right)$ belongs to the Schwartz class. By the inversion formula,

$$g(\boldsymbol{u},\boldsymbol{v})=\hbar^n\operatorname{Tr}\left(\Phi(f)S(\boldsymbol{u},\boldsymbol{v})^{-1}\right)$$

where $f=\mathscr{F}(g)$, so it is sufficient to prove that if

$$\operatorname{Tr}\left(BS(\boldsymbol{u},\boldsymbol{v})^{-1}\right)=0$$

for all $\boldsymbol{u},\boldsymbol{v}\in\mathbb{R}^n$, then $B=0$. Indeed, multiplying by $\overline{f(\boldsymbol{u},\boldsymbol{v})}$ and integrating, we get

$$\operatorname{Tr}BW(f)^*=0$$

for all $f\in\mathscr{S}(\mathbb{R}^{2n})$. Since Schwartz class functions are dense in $L^2(\mathbb{R}^{2n})$, by Lemma 3.1 we get $\operatorname{Tr}BB^*=0$ and, therefore, $B=0$.

Corollary 3.3.

$$\operatorname{Tr}\Phi(f)=\frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^{2n}}f(\boldsymbol{p},\boldsymbol{q})d^n\boldsymbol{p}d^n\boldsymbol{q}$$

Remark. By the Schwartz kernel theorem, the operator $S(\boldsymbol{u},\boldsymbol{v})$ is an integral operator with the distributional kernel

$$e^{\frac{i\hbar}{2}\boldsymbol{u}\boldsymbol{v}-i\boldsymbol{v}\boldsymbol{q}}\delta\left(\boldsymbol{q}-\boldsymbol{q}'-\hbar\boldsymbol{u}\right)$$

so that

$$\operatorname{Tr} S(\boldsymbol{u},\boldsymbol{v})=\left(\frac{2\pi}{\hbar}\right)^{n}\delta(\boldsymbol{u})\delta(\boldsymbol{v})$$

Thus, as is customary in physics texts,

$$\operatorname{Tr}\Phi(f)=\hbar^{-n}\int_{\mathbb{R}^n}\check{f}(\boldsymbol{u},\boldsymbol{v})\delta(\boldsymbol{u})\delta(\boldsymbol{v})d^n\boldsymbol{u}d^n\boldsymbol{v}=\hbar^{-n}\check{f}(0,0)$$

Let $\mathcal{A}_0=\mathscr{S}\left(\mathbb{R}^{2n},\mathbb{R}\right)\subset\mathcal{A}$ be the subalgebra of classical observables on $\mathbb{R}^{2n}$ of rapid decay, and let $\mathscr{A}_0=\mathscr{A}\cap\mathscr{L}(\mathscr{H})$ be the space of bounded quantum observables.

Proposition 3.2. The mapping $\mathcal{A}_0\ni f\mapsto\Phi(f)\in\mathscr{A}_0$ is a quantization, i.e., it satisfies

$$\lim_{\hbar\to0}\frac{1}{2}\Phi^{-1}\left(\Phi\left(f_1\right)\Phi\left(f_2\right)+\Phi\left(f_2\right)\Phi\left(f_1\right)\right)=f_1f_2$$

and the correspondence principle

$$\lim_{\hbar\to0}\Phi^{-1}\left(\left\{\Phi\left(f_1\right),\Phi\left(f_2\right)\right\}_\hbar\right)=\left\{f_1,f_2\right\},\quad f_1,f_2\in\mathcal{A}_0$$

where

$$\left\{\Phi\left(f_1\right),\Phi\left(f_2\right)\right\}_\hbar=\frac{i}{\hbar}\left[\Phi\left(f_1\right),\Phi\left(f_2\right)\right]\quad\text{and}\quad\left\{f_1,f_2\right\}=\frac{\partial f_1}{\partial\boldsymbol{p}}\frac{\partial f_2}{\partial\boldsymbol{q}}-\frac{\partial f_1}{\partial\boldsymbol{q}}\frac{\partial f_2}{\partial\boldsymbol{p}}$$

are, respectively, the quantum bracket and the Poisson bracket.

Proof. In terms of the product $*_\hbar$ introduced in Section 3.1 we have

$$\Phi^{-1}\left(\Phi\left(f_1\right)\Phi\left(f_2\right)\right)=\mathscr{F}\left(\check{f}_1*_\hbar\check{f}_2\right)$$

and it follows from the property WT4 that

$$\Phi^{-1}\left(\Phi\left(f_1\right)\Phi\left(f_2\right)\right)(\boldsymbol{p},\boldsymbol{q})=\frac{1}{(2\pi)^{2n}}\int_{\mathbb{R}^{2n}}\int_{\mathbb{R}^{2n}}\check{f}_1\left(\boldsymbol{u}_1,\boldsymbol{v}_1\right)\check{f}_2\left(\boldsymbol{u}_2,\boldsymbol{v}_2\right)\cdot e^{\frac{i\hbar}{2}(\boldsymbol{u}_1\boldsymbol{v}_2-\boldsymbol{u}_2\boldsymbol{v}_1)-i(\boldsymbol{u}_1+\boldsymbol{u}_2)\boldsymbol{p}-i(\boldsymbol{v}_1+\boldsymbol{v}_2)\boldsymbol{q}}\boldsymbol{d}^n\boldsymbol{u}_1d^n\boldsymbol{u}_2d^n\boldsymbol{v}_1d^n\boldsymbol{v}_2\tag{3.10}$$

Using the expansion

$$e^{\frac{i\hbar}{2}(\boldsymbol{u}_1\boldsymbol{v}_2-\boldsymbol{u}_2\boldsymbol{v}_1)}=1+\frac{i\hbar}{2}\left(\boldsymbol{u}_1\boldsymbol{v}_2-\boldsymbol{u}_2\boldsymbol{v}_1\right)+O\left(\hbar^2\left(\boldsymbol{u}_1\boldsymbol{v}_2-\boldsymbol{u}_2\boldsymbol{v}_1\right)^2\right)$$

as $\hbar\to0$, and the basic properties of the Fourier transform,

$$\mathscr{F}(\boldsymbol{u}\check{f}(\boldsymbol{u},\boldsymbol{v}))=i\frac{\partial f}{\partial\boldsymbol{p}}(\boldsymbol{p},\boldsymbol{q})\quad\text{and}\quad\mathscr{F}(\boldsymbol{v}\check{f}(\boldsymbol{u},\boldsymbol{v}))=i\frac{\partial f}{\partial\boldsymbol{q}}(\boldsymbol{p},\boldsymbol{q})$$

we get from (3.10) that as $\hbar\to0$,

$$\Phi^{-1}\left(\Phi\left(f_1\right)\Phi\left(f_2\right)\right)(\boldsymbol{p},\boldsymbol{q})=\left(f_1f_2\right)(\boldsymbol{p},\boldsymbol{q})-\frac{i\hbar}{2}\left\{f_1,f_2\right\}(\boldsymbol{p},\boldsymbol{q})+O\left(\hbar^2\right)$$

Using skew-symmetry of the Poisson bracket completes the proof.

The quantization associated with the mapping $\Phi=W\circ\mathscr{F}^{-1}$ is called the Weyl quantization.

The correspondence $f \mapsto \Phi(f)$ can be easily extended to the vector space $\widehat{L^1(\mathbb{R}^{2n})}$ - the image of $L^1(\mathbb{R}^{2n})$ under the Fourier transform, which is a subspace of $C(\mathbb{R}^{2n})$. More generally, for $f \in \mathscr{S}(\mathbb{R}^{2n})'$ - the space of tempered distributions on $\mathbb{R}^{2n}$ - the corresponding kernel

$$K(\boldsymbol{q}, \boldsymbol{q}') = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} f\left(\boldsymbol{p}, \frac{\boldsymbol{q}+\boldsymbol{q}'}{2}\right) e^{\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{q}-\boldsymbol{q}')} d^n\boldsymbol{p} \tag{3.11}$$

considered as a tempered distribution on $\mathbb{R}^n \times \mathbb{R}^n$, is a Schwartz kernel of the linear operator

$$\Phi(f) : \mathscr{S}(\mathbb{R}^n) \to \mathscr{S}(\mathbb{R}^n)'$$

In particular, the constant function $f = 1$ corresponds to the identity operator I with $K(\boldsymbol{q}, \boldsymbol{q}') = \delta(\boldsymbol{q} - \boldsymbol{q}')$. In terms of the kernel $K(\boldsymbol{q}, \boldsymbol{q}')$ the Weyl inversion formula takes the form

$$f(\boldsymbol{p}, \boldsymbol{q}) = \int_{\mathbb{R}^n} K\left(\boldsymbol{q} - \frac{1}{2}\boldsymbol{v}, \boldsymbol{q} + \frac{1}{2}\boldsymbol{v}\right) e^{\frac{i}{\hbar}\boldsymbol{v}\boldsymbol{v}} d^n\boldsymbol{v} \tag{3.12}$$

The distribution $f(\boldsymbol{p}, \boldsymbol{q})$ defined by (3.12) is called the Weyl symbol of the operator in $L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ with the Schwartz kernel $K(\boldsymbol{q}, \boldsymbol{q}')$.

Examples below describe classes of distributions f such that the operators $\Phi(f)$ are essentially self-adjoint unbounded operators on the domain $\mathscr{S}(\mathbb{R}^n) \subset L^2(\mathbb{R}^n, d^n\boldsymbol{q})$.

Example 3.1. Let $f = f(\boldsymbol{q}) \in L^p(\mathbb{R}^n)$ for some $1 \leq p \leq \infty$, or let f be a polynomially bounded function as $|\boldsymbol{q}| \to \infty$. In the distributional sense,

$$\check{f}(\boldsymbol{u}, \boldsymbol{v}) = (2\pi)^{n/2} \delta(\boldsymbol{u}) \check{f}(\boldsymbol{v})$$

so that

$$\begin{aligned} K(\boldsymbol{q}, \boldsymbol{q}') &= \frac{1}{(\hbar\sqrt{2\pi})^n} \int_{\mathbb{R}^n} \delta\left(\frac{\boldsymbol{q} - \boldsymbol{q}'}{\hbar}\right) \check{f}(\boldsymbol{v}) e^{-\frac{i}{2}\boldsymbol{v}(\boldsymbol{q}+\boldsymbol{q}')} d^n\boldsymbol{v} \\ &= \delta(\boldsymbol{q} - \boldsymbol{q}') f\left(\frac{\boldsymbol{q}+\boldsymbol{q}'}{2}\right) = f(\boldsymbol{q}) \delta(\boldsymbol{q} - \boldsymbol{q}'). \end{aligned}$$

Thus the operator $\Phi(f)$ is a multiplication by $f(\boldsymbol{q})$ operator on $L^2(\mathbb{R}^n)$. In particular, coordinates $\boldsymbol{q}$ in classical mechanics correspond to coordinate operators $\boldsymbol{Q}$ in quantum mechanics. Similarly, if $f = f(\boldsymbol{p})$, then $\Phi(f) = f(\boldsymbol{P})$. In particular, momenta $\boldsymbol{p}$ in classical mechanics correspond to the momenta operators $\boldsymbol{P}$ in quantum mechanics.

Example 3.2. Let

$$H_{\mathrm{c}} = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{q})$$

be the Hamiltonian function in classical mechanics. Then $H = \Phi(H_c)$ is the corresponding Hamiltonian operator in quantum mechanics,

$$H = \frac{\boldsymbol{P}^2}{2m} + V(\boldsymbol{Q})$$

In Chapter 3 we give necessary conditions for the operator H to be essentially self-adjoint.

Example 3.3. Here we find $f \in \mathscr{S}(\mathbb{R}^{2n})'$ such that

$$\Phi(f) = P_\psi$$

- a pure state P_ψ, where $\psi \in L^2(\mathbb{R}^n), \|\psi\| = 1$. The projection P_ψ is an integral operator with the kernel $\psi(\boldsymbol{q})\overline{\psi(\boldsymbol{q}')}$, and we get from (3.11),

$$\frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} f\left(\boldsymbol{p},\frac{\boldsymbol{q}+\boldsymbol{q}'}{2}\right)e^{\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{q}-\boldsymbol{q}')}d^n\boldsymbol{p}=\psi(\boldsymbol{q})\overline{\psi\left(\boldsymbol{q}'\right)}.$$

Introducing $\boldsymbol{q}_+=\frac{1}{2}\left(\boldsymbol{q}+\boldsymbol{q}'\right),\boldsymbol{q}_-=\frac{1}{2}\left(\boldsymbol{q}-\boldsymbol{q}'\right)$, we obtain

$$\check{f}\left(\frac{2\boldsymbol{q}_-}{\hbar},\boldsymbol{v}\right)=\hbar^n\int_{\mathbb{R}^n}\psi\left(\boldsymbol{q}_-+\boldsymbol{q}_+\right)\overline{\psi\left(\boldsymbol{q}_+-\boldsymbol{q}_-\right)}e^{i\boldsymbol{v}\boldsymbol{q}_+}d^n\boldsymbol{q}_+,$$

or

$$\check{f}(\boldsymbol{u},\boldsymbol{v})=\hbar^n\int_{\mathbb{R}^n}\psi\left(\boldsymbol{q}+\frac{1}{2}\hbar\boldsymbol{u}\right)\overline{\psi\left(\boldsymbol{q}-\frac{1}{2}\hbar\boldsymbol{u}\right)}e^{i\boldsymbol{v}\boldsymbol{q}}d^n\boldsymbol{q}.$$

Assuming that ψ does not depend on $\hbar$, we get in accordance with Corollary 3.3,

$$\check{\rho}(\boldsymbol{u},\boldsymbol{v})=\lim_{\hbar\to 0}\frac{1}{(2\pi\hbar)^n}\check{f}(\boldsymbol{u},\boldsymbol{v})=\frac{1}{(2\pi)^n}\int_{\mathbb{R}^n}|\psi(\boldsymbol{q})|^2e^{i\boldsymbol{v}\boldsymbol{q}}d^n\boldsymbol{v}.$$

Thus in the classical limit $\hbar\to 0$ the pure state P_ψ in quantum mechanics becomes a mixed state in classical mechanics, given by a probability measure $d\mu=\rho(\boldsymbol{p},\boldsymbol{q})d^n\boldsymbol{p}d^n\boldsymbol{q}$ on $\mathbb{R}^{2n}$ with the density

$$\rho(\boldsymbol{p},\boldsymbol{q})=\delta(\boldsymbol{p})|\psi(\boldsymbol{q})|^2$$

It describes a classical particle at rest ($\boldsymbol{p}=0$) with the distribution of coordinates given by the probability measure $|\psi(\boldsymbol{q})|^2d^n\boldsymbol{q}$ on $\mathbb{R}^n$. When $\psi(\boldsymbol{q})=e^{\frac{i}{\hbar}\boldsymbol{p}_0\boldsymbol{q}}\varphi(\boldsymbol{q})$, where $\varphi(\boldsymbol{q})$ does not depend on $\hbar$, the corresponding density is $\rho(\boldsymbol{p},\boldsymbol{q})=\delta\left(\boldsymbol{p}-\boldsymbol{p}_0\right)|\varphi(\boldsymbol{q})|^2$.

Remark. The Weyl quantization can be considered as a way of defining a function $f(\boldsymbol{P},\boldsymbol{Q})$ of non-commuting operators $\boldsymbol{P}=(P_1,...,P_n)$ and $\boldsymbol{Q}=(Q^1,...,Q^n)$ by setting

$$f(\boldsymbol{P},\boldsymbol{Q})=\Phi(f)$$

In particular, if $f(\boldsymbol{p},\boldsymbol{q})=g(\boldsymbol{p})+h(\boldsymbol{q})$, then

$$f(\boldsymbol{P},\boldsymbol{Q})=g(\boldsymbol{P})+h(\boldsymbol{Q})$$

For $f(\boldsymbol{p},\boldsymbol{q})=\boldsymbol{p}\boldsymbol{q}=p_1q^1+\cdots+p_nq^n$ we get, using (3.11),

$$f(\boldsymbol{P},\boldsymbol{Q})=\frac{\boldsymbol{P}\boldsymbol{Q}+\boldsymbol{Q}\boldsymbol{P}}{2}$$

This shows that the Weyl quantization symmetrizes products of the noncommuting factors $\boldsymbol{P}$ and $\boldsymbol{Q}$. In general, let f be a polynomial function,

$$f(\boldsymbol{p},\boldsymbol{q})=\sum_{|\alpha|,|\beta|\leq N}c_{\alpha\beta}\boldsymbol{p}^\alpha\boldsymbol{q}^\beta, \tag{3.13}$$

where for the multi-indices $\alpha=(\alpha_1,...,\alpha_n)$ and $\beta=(\beta_1,...,\beta_n)$,

$$\boldsymbol{p}^\alpha=p_1^{\alpha_1}...p_n^{\alpha_n},\quad \boldsymbol{q}^\beta=\left(q^1\right)^{\beta_1}...\left(q^n\right)^{\beta_n}$$

and $|\alpha|=\alpha_1+\cdots+\alpha_n,\quad |\beta|=\beta_1+\cdots+\beta_n$. Using (3.11), we get the following formula

$$\Phi(f)=\sum_{|\alpha|,|\beta|\leq N}c_{\alpha\beta}\,\mathrm{Sym}\left(\boldsymbol{P}^\alpha\boldsymbol{Q}^\beta\right) \tag{3.14}$$

Here $\mathrm{Sym}\left(\boldsymbol{P}^\alpha\boldsymbol{Q}^\beta\right)$ is a symmetric product, defined by

$$(\boldsymbol{uP}+\boldsymbol{vQ})^k=\sum_{|\alpha|+|\beta|=k}\frac{k!}{\alpha!\beta!}\boldsymbol{u}^\alpha\boldsymbol{v}^\beta\,\mathrm{Sym}\left(\boldsymbol{P}^\alpha\boldsymbol{Q}^\beta\right) \tag{3.15}$$

where $\boldsymbol{uP}+\boldsymbol{vQ}=u^1P_1+\cdots+u^nP_n+v_1Q^1+\cdots+v_nQ^n$ and

$$\alpha!=\alpha_1!...\alpha_n!,\quad \beta!=\beta_1!...\beta_n!$$

Remark. In addition to the Weyl quantization Φ, consider also the mappings $\Phi_1:\mathscr{S}\left(\mathbb{R}^{2n}\right)\to\mathscr{L}(\mathscr{H})$ and $\Phi_2:\mathscr{S}\left(\mathbb{R}^{2n}\right)\to\mathscr{L}(\mathscr{H})$, defined by

$$\Phi_1(f)=\frac{1}{(2\pi)^n}\int_{\mathbb{R}^{2n}}\check{f}(\boldsymbol{u},\boldsymbol{v})e^{\frac{i\hbar}{2}\boldsymbol{uv}}S(\boldsymbol{u},\boldsymbol{v})d^n\boldsymbol{u}d^n\boldsymbol{v}$$

and

$$\Phi_2(f)=\frac{1}{(2\pi)^n}\int_{\mathbb{R}^{2n}}\check{f}(\boldsymbol{u},\boldsymbol{v})e^{-\frac{i\hbar}{2}\boldsymbol{uv}}S(\boldsymbol{u},\boldsymbol{v})d^n\boldsymbol{u}d^n\boldsymbol{v}$$

where $\check{f}=\mathscr{F}^{-1}(f)$ is the inverse Fourier transform. Though Φ_1 and Φ_2 no longer map $\mathcal{A}_0$ into the real vector space $\mathscr{A}_0$ of bounded quantum observables, they satisfy all the properties in Proposition 3.2. It follows from (3.5) that for $f\in\mathscr{S}\left(\mathbb{R}^{2n}\right)$ the operators $\Phi_1(f)$ and $\Phi_2(f)$ are integral operators with the integral kernels

$$K_1\left(\boldsymbol{q},\boldsymbol{q}'\right)=\frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n}f\left(\boldsymbol{p},\boldsymbol{q}'\right)e^{\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{q}-\boldsymbol{q}')}d^n\boldsymbol{p}$$

and

$$K_2\left(\boldsymbol{q},\boldsymbol{q}'\right)=\frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n}f(\boldsymbol{p},\boldsymbol{q})e^{\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{q}-\boldsymbol{q}')}d^n\boldsymbol{p}$$

respectively. As in the case of the Weyl quantization, these formulas extend the mappings $f\mapsto\Phi_1(f)$ and $f\mapsto\Phi_2(f)$ of the space $\mathscr{S}\left(\mathbb{R}^{2n}\right)'$ of tempered distributions on $\mathbb{R}^{2n}$. In particular, if $f(\boldsymbol{p},\boldsymbol{q})$ is a polynomial function (3.13), then

$$\Phi_1(f)=\sum_{|\alpha|,|\beta|\leq N}c_{\alpha\beta}\boldsymbol{P}^\alpha\boldsymbol{Q}^\beta \tag{3.16}$$

and

$$\Phi_2(f)=\sum_{|\alpha|,|\beta|\leq N}c_{\alpha\beta}\boldsymbol{Q}^\beta\boldsymbol{P}^\alpha. \tag{3.17}$$

Therefore the mapping $f\mapsto\Phi_1(f)$ is called the pq-quantization, and the mapping $f\mapsto\Phi_2(f)$ - the $\boldsymbol{qp}$-quantization. Corresponding inversion formulas are

$$f(\boldsymbol{p},\boldsymbol{q})=\int_{\mathbb{R}^n}K_1(\boldsymbol{q}-\boldsymbol{v},\boldsymbol{q})e^{\frac{i}{\hbar}\boldsymbol{pv}}d^n\boldsymbol{v} \tag{3.18}$$

and

$$f(\boldsymbol{p},\boldsymbol{q})=\int_{\mathbb{R}^n}K_2(\boldsymbol{q},\boldsymbol{q}+\boldsymbol{v})e^{\frac{i}{\hbar}\boldsymbol{pv}}d^n\boldsymbol{v} \tag{3.19}$$

The distribution $f(\boldsymbol{p},\boldsymbol{q})$ defined by (3.18) is called the $\boldsymbol{pq}$-symbol of an operator with the Schwartz kernel $K_1\left(\boldsymbol{q},\boldsymbol{q}'\right)$, and the distribution $f(\boldsymbol{p},\boldsymbol{q})$ defined by (3.19) - the $\boldsymbol{qp}$-symbol of an operator with the Schwartz kernel $K_2\left(\boldsymbol{q},\boldsymbol{q}'\right)$. The $\boldsymbol{qp}$-symbols are commonly used in the theory of pseudodifferential operators. It follows from (3.18) and (3.19) that if $f(\boldsymbol{p},\boldsymbol{q})$ is a $\boldsymbol{pq}$-symbol of the operator $\Phi_1(f)$, then $\overline{f(\boldsymbol{p},\boldsymbol{q})}$ is a $\boldsymbol{qp}$-symbol of the adjoint operator $\Phi_1(f)^*$.

Problem 3.

6. Prove formula (3.14).

Problem 3.

7. Prove formulas (3.16)-(3.17).

Problem 3.

8. Prove that Weyl, pq, and $\boldsymbol{qp}$-quantizations are equivalent. (Hint: Find the relations between Weyl, $\boldsymbol{pq}$, and $\boldsymbol{qp}$-symbols of a given operator.)

3.4. The $\star$-product.

The Weyl quantization $\Phi : \mathscr{S}(\mathbb{R}^{2n}) \to \mathscr{L}(\mathscr{H})$, studied in the previous section, defines a new bilinear operation

$$\star_\hbar : \mathscr{S}\left(\mathbb{R}^{2n}\right) \times \mathscr{S}\left(\mathbb{R}^{2n}\right) \to \mathscr{S}\left(\mathbb{R}^{2n}\right)$$

on $\mathscr{S}(\mathbb{R}^{2n})$ by the formula

$$f_1 \star_\hbar f_2 = \Phi^{-1}\left(\Phi\left(f_1\right)\Phi\left(f_2\right)\right).$$

This operation is called the $\star$-product [26]. According to (3.10),

$$\left(f_1 \star_\hbar f_2\right)(\boldsymbol{p},\boldsymbol{q}) = \frac{1}{(2\pi)^{2n}} \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} \check{f}_1(\boldsymbol{u}_1,\boldsymbol{v}_1)\, \check{f}_2(\boldsymbol{u}_2,\boldsymbol{v}_2)\, . \tag{3.20}$$
$$. \, e^{\frac{i\hbar}{2}(\boldsymbol{u}_1\boldsymbol{v}_2 - \boldsymbol{u}_2\boldsymbol{v}_1) - i(\boldsymbol{u}_1+\boldsymbol{u}_2)\boldsymbol{p} - i(\boldsymbol{v}_1+\boldsymbol{v}_2)\boldsymbol{q}} d^n\boldsymbol{u}_1 d^n\boldsymbol{u}_2 d^n\boldsymbol{v}_1 d^n\boldsymbol{v}_2.$$

The *-product on $\mathscr{S}(\mathbb{R}^{2n})$ has the following properties.

1. Associativity:

$$f_1 \star_\hbar (f_2 \star_\hbar f_3) = (f_1 \star_\hbar f_2) \star_\hbar f_3.$$

2. Semi-classical limit:

$$\left(f_1 \star_\hbar f_2\right)(\boldsymbol{p},\boldsymbol{q}) = \left(f_1 f_2\right)(\boldsymbol{p},\boldsymbol{q}) - \frac{i\hbar}{2}\left\{f_1, f_2\right\}(\boldsymbol{p},\boldsymbol{q}) + O\left(\hbar^2\right) \text{ as } \hbar \to 0$$

3. Property of the unit:

$$f \star_\hbar \mathbf{1} = \mathbf{1} \star_\hbar f,$$

where 1 is a function which identically equals 1 on $\mathbb{R}^{2n}$.

4. The cyclic trace property:

$$\tau\left(f_1 \star_\hbar f_2\right) = \tau\left(f_2 \star_\hbar f_1\right)$$

where the $\mathbb{C}$-linear map $\tau : \mathscr{S}\left(\mathbb{R}^{2n}\right) \to \mathbb{C}$ is defined by

$$\tau(f) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} f(\boldsymbol{p}, \boldsymbol{q}) d^n\boldsymbol{p} d^n\boldsymbol{q}$$

Property 1 follows from the corresponding property for the product $*_\hbar$ (see Section 3.1), property 2 follows from Proposition 3.2, and properties 3 and 4 directly follow from the definition (3.20). The complex vector space $\mathscr{S}\left(\mathbb{R}^{2n}\right) \oplus \mathbb{C}1$ with the bilinear operation $\star_\hbar$ is an associative algebra over $\mathbb{C}$ with unit 1 and the cyclic trace τ, satisfying the correspondence principle,

$$\lim_{\hbar\to 0} \frac{i}{\hbar}\left(f_1 \star_\hbar f_2 - f_2 \star_\hbar f_1\right) = \{f_1, f_2\}\,.$$

Consider the tensor product of Hilbert spaces

$$L^2\left(\mathbb{R}^{2n}\right) \otimes L^2\left(\mathbb{R}^{2n}\right) \simeq L^2\left(\mathbb{R}^{2n} \times \mathbb{R}^{2n}\right)$$

and define the unitary operator $\boldsymbol{U}_1$ on $L^2\left(\mathbb{R}^{2n}\right) \otimes L^2\left(\mathbb{R}^{2n}\right)$ by

$$\boldsymbol{U}_1 = e^{-\frac{i\hbar}{2}\left(\frac{\partial}{\partial \boldsymbol{p}} \otimes \frac{\partial}{\partial \boldsymbol{q}}\right)}$$

where

$$\frac{\partial}{\partial \boldsymbol{p}} \otimes \frac{\partial}{\partial \boldsymbol{q}} = \sum_{k=1}^{n} \frac{\partial}{\partial p_k} \otimes \frac{\partial}{\partial q^k}$$

It follows from the theory of Fourier transform that for $f_1, f_2 \in \mathscr{S}\left(\mathbb{R}^{2n}\right)$,

$$\left(\boldsymbol{U}_1\left(f_1 \otimes f_2\right)\right)\left(\boldsymbol{p}_1, \boldsymbol{q}_1, \boldsymbol{p}_2, \boldsymbol{q}_2\right) = \frac{1}{(2\pi)^{2n}} \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} \check{f}_1\left(\boldsymbol{u}_1, \boldsymbol{v}_1\right) \check{f}_2\left(\boldsymbol{u}_2, \boldsymbol{v}_2\right).$$
$$\cdot e^{\frac{i\hbar}{2}\boldsymbol{u}_1\boldsymbol{v}_2 - i\boldsymbol{u}_1\boldsymbol{p}_1 - i\boldsymbol{u}_2\boldsymbol{p}_2 - i\boldsymbol{v}_1\boldsymbol{q}_1 - i\boldsymbol{v}_2\boldsymbol{q}_2} d^n\boldsymbol{u}_1 d^n\boldsymbol{u}_2 d^n\boldsymbol{v}_1 d^n\boldsymbol{v}_2$$

Similarly, defining the unitary operator $\boldsymbol{U}_2$ on $L^2\left(\mathbb{R}^{2n}\right) \otimes L^2\left(\mathbb{R}^{2n}\right)$ by

$$\boldsymbol{U}_2 = e^{-\frac{i\hbar}{2}\left(\frac{\partial}{\partial \boldsymbol{q}} \otimes \frac{\partial}{\partial p}\right)}$$

we get

$$\left(\boldsymbol{U}_2\left(f_1 \otimes f_2\right)\right)\left(\boldsymbol{p}_1, \boldsymbol{q}_1, \boldsymbol{p}_2, \boldsymbol{q}_2\right) = \frac{1}{(2\pi)^{2n}} \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} \check{f}_1\left(\boldsymbol{u}_1, \boldsymbol{v}_1\right) \check{f}_2\left(\boldsymbol{u}_2, \boldsymbol{v}_2\right)$$
$$\cdot e^{\frac{i\hbar}{2}\boldsymbol{u}_2\boldsymbol{v}_1 - i\boldsymbol{u}_1\boldsymbol{p}_1 - i\boldsymbol{u}_2\boldsymbol{p}_2 - i\boldsymbol{v}_1\boldsymbol{q}_1 - \boldsymbol{v}_2\boldsymbol{q}_2} d^n\boldsymbol{u}_1 d^n\boldsymbol{u}_2 d^n\boldsymbol{v}_1 d^n\boldsymbol{v}_2$$

Finally, define the unitary operator $\boldsymbol{U}_\hbar$ on $L^2\left(\mathbb{R}^{2n}\right) \otimes L^2\left(\mathbb{R}^{2n}\right)$ by

$$\boldsymbol{U}_\hbar = \boldsymbol{U}_1\boldsymbol{U}_2^{-1} = e^{-\frac{i\hbar}{2}\left(\frac{\partial}{\partial \boldsymbol{p}} \otimes \frac{\partial}{\partial \boldsymbol{q}} - \frac{\partial}{\partial \boldsymbol{q}} \otimes \frac{\partial}{\partial \boldsymbol{p}}\right)}$$

and denote by $m : \mathscr{S}\left(\mathbb{R}^{2n}\right) \otimes \mathscr{S}\left(\mathbb{R}^{2n}\right) \to \mathscr{S}\left(\mathbb{R}^{2n}\right)$ the point-wise product of functions, $\left(m\left(f_1 \otimes f_2\right)\right)\left(\boldsymbol{p}, \boldsymbol{q}\right) = f_1(\boldsymbol{p}, \boldsymbol{q}) f_2(\boldsymbol{p}, \boldsymbol{q})$. Then the $\star$-product can be written in the following concise form:

$$f_1 \star_\hbar f_2 = \left(m \circ \boldsymbol{U}_\hbar\right)\left(f_1 \otimes f_2\right). \tag{3.21}$$

[026] Also called Moyal product in physics.

In analogy with the Poisson bracket $\{,\} on \mathbb{R}^{2n}$ associated with the canonical symplectic form $\omega = d\boldsymbol{p} \wedge d\boldsymbol{q}$,

$$\{f_1, f_2\} = \frac{\partial f_1}{\partial \boldsymbol{p}} \frac{\partial f_2}{\partial \boldsymbol{q}} - \frac{\partial f_1}{\partial \boldsymbol{q}} \frac{\partial f_2}{\partial \boldsymbol{p}}$$

we introduce the notation

$$\{\overset{\otimes}{,}\} = \frac{\partial}{\partial \boldsymbol{p}} \otimes \frac{\partial}{\partial \boldsymbol{q}} - \frac{\partial}{\partial \boldsymbol{q}} \otimes \frac{\partial}{\partial \boldsymbol{p}} = \frac{\partial^2}{\partial \boldsymbol{p}_1 \partial \boldsymbol{q}_2} - \frac{\partial^2}{\partial \boldsymbol{q}_1 \partial \boldsymbol{p}_2}.$$

Then it follows from the theory of Fourier transform that formula (3.21) for the $*$-product can be rewritten as

$$\left(f_1 \star_\hbar f_2\right)(\boldsymbol{p}, \boldsymbol{q}) = \left(e^{-\frac{i\hbar}{2}\{\overset{\otimes}{P}\}} f_1\left(\boldsymbol{p}_1, \boldsymbol{q}_1\right) f_2\left(\boldsymbol{p}_2, \boldsymbol{q}_2\right) \right)\Big|_{\substack{\boldsymbol{p}_1=\boldsymbol{p}_2=\boldsymbol{p} \\ \boldsymbol{q}_1=\boldsymbol{q}_2=\boldsymbol{q}}}. \tag{3.22}$$

Thus we have shown that on $\mathscr{S}\left(\mathbb{R}^{2n}\right)$ the $\star$-product can be equivalently defined by (3.20), or by (3.21) and (3.22). The latter representation has the advantage that the formal expansion of the exponential $e^{-\frac{i\hbar}{2}\{\overset{\otimes}{,}\}}$ into the power series gives the asymptotic expansion of the $\star$-product as $\hbar \to 0$. Namely, define the bidifferential operators

$$B_k : \mathscr{S}\left(\mathbb{R}^{2n}\right) \otimes \mathscr{S}\left(\mathbb{R}^{2n}\right) \to \mathscr{S}\left(\mathbb{R}^{2n}\right)$$

by $B_k = m \circ \{\overset{\otimes}{,}\}^k$ for $k \geq 1$ and $B_0 = m$.

Lemma 3.2. For every $f_1, f_2 \in \mathscr{S}\left(\mathbb{R}^{2n}\right)$ and $l \in \mathbb{N}$ there is $C > 0$ such that for all $\boldsymbol{p}, \boldsymbol{q} \in \mathbb{R}^{2n}$

$$\left| \left(f_1 \star_\hbar f_2\right)(\boldsymbol{p}, \boldsymbol{q}) - \sum_{k=0}^{l} \frac{(-i\hbar)^k}{2^k k!} B_k\left(f_1, f_2\right)(\boldsymbol{p}, \boldsymbol{q}) \right| \leq C\hbar^{l+1} \quad \text{as} \quad \hbar \to 0$$

Succinctly,

$$\left(f_1 \star_\hbar f_2\right)(\boldsymbol{p}, \boldsymbol{q}) = \sum_{k=0}^{\infty} \frac{(-i\hbar)^k}{2^k k!} B_k\left(f_1, f_2\right)(\boldsymbol{p}, \boldsymbol{q}) + O\left(\hbar^\infty\right). \tag{3.23}$$

Proof. Expanding the exponential function $e^{\frac{i\hbar}{2}(\boldsymbol{u}_1 \boldsymbol{v}_2 - \boldsymbol{u}_2 \boldsymbol{v}_1)}$ into the power series and repeating the proof of Proposition 3.2 gives the result.

Finally, we get another integral representation for the $\star$-product. Applying the Fourier inversion formula to the integral over $d^n\boldsymbol{u}_1 d^n\boldsymbol{v}_1$ in (3.20), we get

$$\begin{aligned}
\left(f_1 \star_\hbar f_2\right)(\boldsymbol{p}, \boldsymbol{q}) &= \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} f_1\left(\boldsymbol{p} - \frac{\hbar}{2}\boldsymbol{v}_2, \boldsymbol{q} + \frac{\hbar}{2}\boldsymbol{u}_2\right) \check{f}_2\left(\boldsymbol{u}_2, \boldsymbol{v}_2\right) \\
&= \frac{1}{(2\pi)^{2n}} \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} f_1\left(\boldsymbol{p} - \frac{\hbar}{2}\boldsymbol{v}_2, \boldsymbol{q} + \frac{\hbar}{2}\boldsymbol{u}_2\right) f_2\left(\boldsymbol{p}_2, \boldsymbol{q}_2\right) \\
&\quad \cdot e^{-i\boldsymbol{u}_2\boldsymbol{p} - i\boldsymbol{v}_2\boldsymbol{q}} d^n\boldsymbol{u}_2 d^n\boldsymbol{v}_2 - i\boldsymbol{v}_2\boldsymbol{q} + i\boldsymbol{u}_2\boldsymbol{p}_2 + i\boldsymbol{v}_2\boldsymbol{q}_2 \\
&\quad d^n\boldsymbol{p}_2 d^n\boldsymbol{q}_2 d^n\boldsymbol{u}_2 d^n\boldsymbol{v}_2
\end{aligned}$$

and changing variables $\boldsymbol{p}_1 = \boldsymbol{p} - \frac{\hbar}{2}\boldsymbol{v}_2, \boldsymbol{q}_1 = \boldsymbol{q} + \frac{\hbar}{2}\boldsymbol{u}_2$, we obtain

$$\begin{aligned}
\left(f_1 \star_\hbar f_2\right)(\boldsymbol{p}, \boldsymbol{q}) &= \frac{1}{(\pi\hbar)^{2n}} \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} f_1\left(\boldsymbol{p}_1, \boldsymbol{q}_1\right) f_2\left(\boldsymbol{p}_2, \boldsymbol{q}_2\right). \\
&\quad \cdot e^{\frac{2i}{\hbar}(\boldsymbol{p}_1\boldsymbol{q} - \boldsymbol{p}\boldsymbol{q}_1 + \boldsymbol{q}_1\boldsymbol{p}_2 - \boldsymbol{q}_2\boldsymbol{p}_1 + \boldsymbol{p}\boldsymbol{q}_2 - \boldsymbol{p}_2\boldsymbol{q})} d^n\boldsymbol{p}_1 d^n\boldsymbol{q}_1 d^n\boldsymbol{p}_2 d^n\boldsymbol{q}_2.
\end{aligned}$$

Let $\triangle$ be a Euclidean triangle (a 2 -simplex) in the phase space $\mathbb{R}^{2n}$ with the vertices $(\boldsymbol{p},\boldsymbol{q}),(\boldsymbol{p}_1,\boldsymbol{q}_1)$, and $(\boldsymbol{p}_2,\boldsymbol{q}_2)$. It is easy to see that

$$\boldsymbol{p}_1\boldsymbol{q}-\boldsymbol{p}\boldsymbol{q}_1+\boldsymbol{q}_1\boldsymbol{p}_2-\boldsymbol{q}_2\boldsymbol{p}_1+\boldsymbol{p}\boldsymbol{q}_2-\boldsymbol{p}_2\boldsymbol{q}=2\int_{\triangle}\omega$$

which is twice the symplectic area of $\triangle$ - the sum of oriented areas of the projections of $\triangle$ onto two-dimensional planes $(p_1,q^1),...,(p_n,q^n)$. Thus we have the final formula

$$\begin{aligned}(f_1\star_\hbar f_2)(\boldsymbol{p},\boldsymbol{q})=\frac{1}{(\pi\hbar)^{2n}}\int_{\mathbb{R}^{2n}}\int_{\mathbb{R}^{2n}}f_1(\boldsymbol{p}_1,\boldsymbol{q}_1)\,f_2(\boldsymbol{p}_2,\boldsymbol{q}_2)\\ \cdot e^{\frac{4i}{\hbar}\int_{\triangle}\omega}d^n\boldsymbol{p}_1d^n\boldsymbol{q}_1d^n\boldsymbol{p}_2d^n\boldsymbol{q}_2\end{aligned}\tag{3.24}$$

which is a composition formula for the Weyl symbols.
Remark. It is instructive to compare formulas (3.23) and (3.24). The latter formula represents the $\star$-product on $\mathscr{S}(\mathbb{R}^{2n})$ as an absolutely convergent integral, and is equivalent to the Weyl quantization. The former formula is an asymptotic expansion of the $\star$-product as $\hbar\to 0$, and does not capture all properties of the Weyl quantization. In general, the power series in (3.23) diverges; for polynomial functions this series becomes a finite sum and gives a formula for the $\star$-product of polynomials.

Problem 3.

9 (Composition formula for $\boldsymbol{pq}$-symbols). Let $f_1(\boldsymbol{p},\boldsymbol{q})$ and $f_2(\boldsymbol{p},\boldsymbol{q})$ be, respectively, the $\boldsymbol{pq}$-symbols of the operators $\Phi_1(f_1)$ and $\Phi_1(f_2)$. Show that the pq-symbol of the operator $\Phi_1(f_1)\Phi_1(f_2)$ is given by

$$f(\boldsymbol{p},\boldsymbol{q})=\frac{1}{(2\pi h)^n}\int_{\mathbb{R}^{2n}}f_1(\boldsymbol{p},\boldsymbol{q}_1)\,f_2(\boldsymbol{p}_1,\boldsymbol{q})\,e^{\frac{i}{\hbar}(\boldsymbol{p}-\boldsymbol{p}_1)(\boldsymbol{q}-\boldsymbol{q}_1)}d^n\boldsymbol{p}_1d^n\boldsymbol{q}_1.$$

(Hint: Use the formula for $(m\circ\boldsymbol{U}_1^2)(f_1\otimes f_2)$.)

Problem 3.

10 (Composition formula for $\boldsymbol{qp}$-symbols). Let $f_1(\boldsymbol{p},\boldsymbol{q})$ and $f_2(\boldsymbol{p},\boldsymbol{q})$ be, respectively, the $\boldsymbol{qp}$-symbols of the operators $\Phi_2(f_1)$ and $\Phi_2(f_2)$. Show that the qp-symbol of the operator $\Phi_2(f_1)\Phi_2(f_2)$ is given by

$$f(\boldsymbol{p},\boldsymbol{q})=\frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^{2n}}f_1(\boldsymbol{p}_1,\boldsymbol{q})\,f_2(\boldsymbol{p},\boldsymbol{q}_1)\,e^{-\frac{i}{\hbar}(\boldsymbol{p}-\boldsymbol{p}_1)(\boldsymbol{q}-\boldsymbol{q}_1)}d^n\boldsymbol{p}_1d^n\boldsymbol{q}_1$$

(Hint: Use the formula for $\left(m\circ\boldsymbol{U}_2^{-2}\right)(f_1\otimes f_2)$.)

Problem 3.

11. Using (3.24) prove that the $\star$-product is associative.

Problem 3.

12. For classical observable $f(\boldsymbol{p},\boldsymbol{q})$ define the $\star$-exponential (the analog of the evolution operator) by

$$\exp_\star f = \sum_{n=0}^{\infty} \frac{\hbar^{-n}}{n!} \underbrace{f \star_\hbar f \star_\hbar \cdots \star_\hbar f}_{n}.$$

Compute $\exp_\star(-itH_{\rm c})$, where $H_{\rm c}(\boldsymbol{p},\boldsymbol{q})$ is the Hamiltonian function (2.27) of the harmonic oscillator.

4.2.3 3. Weyl Relations 3: Deformation quantization

3.5. Deformation quantization.

Here we consider the quantization procedure from a formal algebraic point of view as the deformation theory of associative algebras. Let $\mathcal{A}$ be a $\mathbb{C}$-algebra (or an associative algebra with unit over a field k of characteristic zero) with a bilinear multiplication map $m_0 : \mathcal{A} \otimes_{\mathbb{C}} \mathcal{A} \to \mathcal{A}$, which we will abbreviate as $a \cdot b = m_0(a,b)$. Denote by $\mathbb{C}[[t]]$ the ring of formal power series in t with coefficients in $\mathbb{C}$,

$$\mathbb{C}[[t]] = \left\{ \sum_{n=0}^{\infty} a_n t^n : a_n \in \mathbb{C} \right\},$$

and let

$$\mathcal{A}_t = \mathbb{C}[[t]] \otimes_{\mathbb{C}} \mathcal{A}$$

be the $\mathbb{C}[[t]]$-algebra of formal power series in t with coefficients in $\mathcal{A}$. The multiplication in $\mathcal{A}_t$ is a $\mathbb{C}[[t]]$-bilinear extension of the multiplication in $\mathcal{A}$, which we continue to denote by m_0. The algebra $\mathcal{A}_t$ is $\mathbb{Z}$-graded,

$$\mathcal{A}_t = \bigoplus_{n=0}^{\infty} A_n,$$

where $A_n = t^n \mathcal{A}$, so that $A_m \cdot A_m \subset A_{m+n}$.

Definition. A formal deformation of a $\mathbb{C}$-algebra $\mathcal{A}$ with a multiplication m_0 is an associative algebra $\mathcal{A}_t$ over the ring $\mathbb{C}[[t]]$ with a $\mathbb{C}[[t]]$-bilinear multiplication map $m_t : \mathcal{A}_t \otimes_{\mathbb{C}[[t]]} \mathcal{A}_t \to \mathcal{A}_t$ such that

$$m_t(a,b) = a \cdot b + \sum_{n=1}^{\infty} t^n m_n(a,b)$$

for all $a, b \in \mathcal{A}$, where $m_n : \mathcal{A} \otimes_{\mathbb{C}} \mathcal{A} \to \mathcal{A}$ are bilinear mappings.
It follows from $\mathbb{C}[[t]]$-bilinearity of m_t that the associativity condition is equivalent to

$$m_t\left(m_t(a,b),c\right) = m_t\left(a, m_t(b,c)\right) \tag{3.25}$$

for all $a, b, c \in \mathcal{A}$.

Definition. Two formal deformations m_t and $\tilde{m}_t$ of a $\mathbb{C}$-algebra $\mathcal{A}$ are equivalent if there is a $\mathbb{C}[[t]]$-linear mapping $F_t : \mathcal{A}_t \to \mathcal{A}_t$ such that
(i) for every $a \in \mathcal{A}$,

$$F_t(a) = a + \sum_{n=1}^{\infty} t^n f_n(a)$$

where $f_n : \mathcal{A} \to \mathcal{A}$ are linear mappings;
(ii) for all $a, b \in \mathcal{A}$,

$$F_t\left(\tilde{m}_t(a,b)\right) = m_t\left(F_t(a), F_t(b)\right)$$

The bilinear maps m_n satisfy infinitely many relations which are obtained by expanding (3.25) into formal power series in t. The first two of them, arising from comparing the coefficients at t and t^2, are

$$a \cdot m_1(b,c) - m_1(a \cdot b, c) + m_1(a, b \cdot c) - m_1(a,b) \cdot c = 0,$$

and

$$\begin{aligned} a \cdot m_2(b,c) - m_2(a \cdot b, c) + m_2(a, b \cdot c) - m_2(a,b) \cdot c \\ = m_1\left(m_1(a,b), c\right) - m_1\left(a, m_1(b,c)\right). \end{aligned}$$

In general

$$\begin{aligned} a \cdot m_n(b,c) - m_n(a \cdot b, c) + m_n(a, b \cdot c) - m_n(a,b) \cdot c \\ = \sum_{j=1}^{n-1} \left(m_j\left(m_{n-j}(a,b), c\right) - m_j\left(a, m_{n-j}(b,c)\right)\right). \end{aligned}$$

The main tool for understanding these equations and studying the deformation theory of associative algebras is the Hochschild cohomology. Namely, let M be an $\mathcal{A}$-bimodule, i.e., a left and right module for the $\mathbb{C}$-algebra $\mathcal{A}$.

Definition. The Hochschild cochain complex $C^\bullet(\mathcal{A}, M)$ of a $\mathbb{C}$-algebra $\mathcal{A}$ with coefficients in $\mathcal{A}$-bimodule M is defined by the cochains

$$\mathbb{C}^n(\mathcal{A}, M) = \mathrm{Hom}_{\mathbb{C}}\left(\mathcal{A}^{\otimes n}, M\right)$$

i.e., n-linear maps $f\left(a_1, ..., a_n\right)$ on $\mathcal{A}$ with values in M, and the differential $d_n : C^n(\mathcal{A}, M) \to C^{n+1}(\mathcal{A}, M)$,

$$\begin{aligned} \left(d_n f\right)\left(a_1, a_2, ..., a_{n+1}\right) =& a_1 \cdot f\left(a_2, ..., a_{n+1}\right) \\ &+ \sum_{j=1}^{n} (-1)^j f\left(a_1, ..., a_{j-1,}, a_j \cdot a_{j+1}, a_{j+2}..., a_{n+1}\right) \\ &+ (-1)^{n+1} f\left(a_1, ..., a_n\right) \cdot a_{n+1} \end{aligned}$$

We have $d^2 = 0$, i.e., $d_{n+1} \circ d_n = 0$, and the cohomology $H^\bullet(\mathcal{A}, M)$ of the complex $(\mathrm{C}^\bullet(\mathcal{A}, M), d)$,

$$H^n(\mathcal{A}, M) = \ker d_n / \operatorname{Im} d_{n-1}$$

is called the Hochschild cohomology of the algebra $\mathcal{A}$ with coefficients in the $\mathcal{A}$-bimodule M.

In the deformation theory of associative algebras we have the simplest non-trivial case $M = \mathcal{A}$ with the left and right $\mathcal{A}$-actions given by the multiplication map. The associativity equation (3.25) can be written as

$$(d_2 m_1)(a,b,c) = 0$$
$$(d_2 m_n)(a,b,c) = \sum_{j=1}^{n-1} \left(m_j\left(m_{n-j}(a,b),c\right) - m_j\left(a, m_{n-j}(b,c)\right)\right), \quad a,b,c \in \mathcal{A}$$

It is quite remarkable that the Hochschild cochain complex $C^\bullet(\mathcal{A},\mathcal{A})$ carries an additional structure of a graded Lie algebra, which plays a fundamental
role in studying the associativity equation (3.25). Namely, for $f \in \mathrm{C}^m(\mathcal{A},\mathcal{A})$ and $g \in \mathbb{C}^n(\mathcal{A},\mathcal{A})$ let

$$(f \circ g)(a_1, ..., a_{m+n-1})$$
$$= \sum_{j=0}^{m-1} (-1)^j f\left(a_1, ..., a_j, g\left(a_{j+1}, ..., a_{j+n}\right), a_{j+n+1}, ..., a_{m+n-1}\right),$$

and define

$$[f,g]_G = f \circ g - (-1)^{(m-1)(n-1)} g \circ f.$$

The linear mapping $[,]_G : \mathrm{C}^m(\mathcal{A},\mathcal{A}) \times \mathrm{C}^n(\mathcal{A},\mathcal{A}) \to \mathbb{C}^{m+n-1}(\mathcal{A},\mathcal{A})$ satisfies $[f,g]_G = -(-1)^{(m-1)(n-1)}[g,f]_G$, and is called the Gerstenhaber bracket [27]. Considering the restriction of a multiplication m_t to $\mathcal{A} \otimes_{\mathbb{C}} \mathcal{A}$ as formal power series in t with coefficients in $C^\bullet(\mathcal{A},\mathcal{A})$ and using the Gerstenhaber bracket, we can rewrite (3.25) in the succinct form:

$$[m_t, m_t]_G = 0. \tag{3.26}$$

Let $\mathcal{A}$ be a commutative $\mathbb{C}$-algebra, and let $\mathcal{A}_t$ be a formal deformation of $\mathcal{A}$. Define the bilinear map $\{\} :, \mathcal{A} \otimes \mathbb{C}\mathcal{A} \to \mathcal{A}$ by

$$\{a,b\} = m_1(a,b) - m_1(b,a), \quad a,b \in \mathcal{A} \tag{3.27}$$

Lemma 3.3. *A formal deformation $\mathcal{A}_t$ of a commutative $\mathbb{C}$-algebra $\mathcal{A}$ equips $\mathcal{A}$ with a Poisson algebra structure with the bracket $\{,\}$.*

Proof. Consider the equation $d\mu_1(a,b,c) = 0$. Subtracting from it the equation with a and c interchanged, and using the commutativity of $\mathcal{A}$, we obtain

$$\{a \cdot b, c\} - \{a, b \cdot c\} = a \cdot \{b,c\} - c \cdot \{a,b\}.$$

Interchanging b and c, we get

$$\{a \cdot c, b\} - \{a, b \cdot c\} = a \cdot \{c,b\} - b \cdot \{a,c\}$$

and interchanging further a and c, we obtain

$$\{a \cdot c, b\} - \{c, a \cdot b\} = c \cdot \{a,b\} - b \cdot \{c,a\}.$$

Adding the first and third equations and subtracting the second equation gives

$$\{a \cdot b, c\} = a \cdot \{a,c\} + b \cdot \{a,c\}$$

so that the skew-symmetric cochain $\{,\} \in C^2(\mathcal{A},\mathcal{A})$ satisfies the Leibniz rule. To prove the Jacobi identity, observe that

$$\{a,b\} = \frac{m_t(a,b) - m_t(b,a)}{t} \bmod t\mathcal{A}_t. \tag{3.28}$$

Using associativity condition (3.25) (associativity modulo $t^2\mathcal{A}_t$ is sufficient) we get

$$\begin{gathered}\{\{a,b\},c\} + \{\{c,a\},b\} + \{\{b,c\},a\} = \frac{1}{t^2}\left(\left(m_t\left(m_t(a,b) - m_t(b,a)\right),c\right)\right.\\ -m_t\left(c, m_t(a,b) - m_t(b,a)\right) + m_t\left(m_t(c,a) - m_t(a,c),b\right)\\ -m_t\left(b, m_t(c,a) - m_t(a,c)\right) + m_t\left(m_t(b,c) - m_t(c,b),a\right)\\ \left.-m_t\left(a, m_t(b,c) - m_t(c,b)\right)\right) \bmod t\mathcal{A}_t = 0\end{gathered}$$

This result motivates the following definition.

Definition. A deformation quantization of a Poisson algebra $(\mathcal{A},\{\},)with$ the commutative product $m_0 : \mathcal{A}\otimes_{\mathbb{C}}\mathcal{A}\to\mathcal{A}$ is a formal deformation $\mathcal{A}_t$ of an algebra $\mathcal{A}$ such that the multiplication map m_t satisfies (3.28).

By Lemma 3.3, every formal deformation $\mathcal{A}_t$ of a commutative algebra $\mathcal{A}$ is a deformation quantization of the Poisson algebra $(\mathcal{A},\{\},)withthe$ Poisson bracket given by (3.27).

According to Lemma 3.2, a deformation quantization of the Poisson algebra $(\mathscr{S}(\mathbb{R}^{2n}),\{\},)$, where the Poisson bracket is associated with the canonical symplectic form $\omega = d\boldsymbol{p}\wedge d\boldsymbol{q}$, is the algebra $\mathscr{S}(\mathbb{R}^{2n})[[t]]$, where $t = -i\hbar$ and $\hbar$ is considered as a formal parameter, and the multiplication map is given by the $\star$-product. The following statement is a formal algebraic analog of the representation (3.22) for the $\star$-product.

Theorem 3.4 (Universal deformation). Let $\mathcal{A}$ be a commutative $\mathbb{C}$-algebra with the multiplication map m_0, and let φ_1 and φ_2 be two commuting derivations of $\mathcal{A}$, i.e., linear maps $\varphi_1,\varphi_2 : \mathcal{A}\to\mathcal{A}$ satisfying Leibniz rule and

$$\varphi_1\circ\varphi_2 = \varphi_2\circ\varphi_1.$$

Then

$$\{a,b\} = \varphi_1(a)\cdot\varphi_2(b) - \varphi_2(a)\cdot\varphi_1(b),\quad a,b\in\mathcal{A},$$

defines a Poisson bracket on $\mathcal{A}$, and the formula

$$m_t = m_0\circ e^{t\Phi},\quad \Phi = \varphi_1\otimes\varphi_2$$

called the universal deformation formula, gives a deformation quantization of the Poisson algebra $(\mathcal{A},\{\},)$.

Proof. The Jacobi identity for the bracket $\{,\}follows fromthecommu$ - tativity of the derivations φ_1 and φ_2. To show that $\mathcal{A}_t$ is a deformation quantization of the Poisson algebra $(\mathcal{A},\{,\}),weneedtoverifytheasso$ - ciativity condition (3.25) for the map m_t. Let $\Delta : \mathcal{A}\to\mathcal{A}\otimes\mathbb{C}\mathcal{A}$ be the coproduct map,

$$\Delta(a) = a\otimes 1 + 1\otimes a,\quad a\in\mathcal{A}$$

It extends to a $\mathbb{C}$-linear mapping from $\mathrm{Hom}_{\mathbb{C}}(\mathcal{A},\mathcal{A})$ to $\mathrm{Hom}_{\mathbb{C}}(\mathcal{A}^{\otimes 2},\mathcal{A}^{\otimes 2})$, which we continue to denote by Δ, and

$$\Delta(\varphi) = \varphi\otimes\mathrm{id} + \mathrm{id}\otimes\varphi,\quad \varphi\in\mathrm{Hom}_{\mathbb{C}}(\mathcal{A},\mathcal{A}).$$

[027] Together with the cup product of cochains, the Gerstenhaber bracket equips $C^*(\mathcal{A},\mathcal{A})$ with the structure of a Gerstenhaber algebra.

To prove (3.25), we observe that the Leibniz rule and the binomial formula yield the following identity for a derivation φ of $\mathcal{A}$:

$$e^{t\varphi} \circ m_0 = m_0 \circ e^{t\Delta(\varphi)}.$$

Using commutativity of φ_1 and φ_2, we obtain

$$\begin{aligned} m_t\left(a, m_t(b,c)\right) &= m_0\left(e^{t\Phi}\left(a \otimes m_0\left(e^{t\Phi}(b\otimes c)\right)\right)\right) \\ &= \left(m_0 \circ (\mathrm{id}\otimes m_0)\right)\left(e^{t(\mathrm{id}\otimes\Delta)(\Phi)} e^{t\mathrm{id}\otimes\Phi}(a\otimes b\otimes c)\right) \\ &= \left(m_0 \circ (\mathrm{id}\otimes m_0)\right)\left(e^{t(\mathrm{id}\otimes\Delta)(\Phi)+t\mathrm{id}\otimes\Phi}(a\otimes b\otimes c)\right) \end{aligned}$$

where $(\mathrm{id}\otimes\Delta)(\Phi) = \varphi_1 \otimes \Delta(\varphi_2) \in \mathcal{A}^{\otimes 3}$. Similarly,

$$m_t\left(m_t(a,b),c\right) = \left(m_0 \circ (m_0\otimes \mathrm{id})\right)\left(e^{t(\Delta\otimes\mathrm{id})(\Phi)+t\Phi\otimes\mathrm{id}}(a\otimes b\otimes c)\right)$$

where $(\Delta\otimes\mathrm{id})(\Phi) = \Delta(\varphi_1)\otimes\varphi_2 \in \mathcal{A}^{\otimes 3}$. Since $m_0\circ(\mathrm{id}\otimes m_0) = m_0\circ(m_0\otimes\mathrm{id})$, the associativity of the multiplication m_t is equivalent to

$$(\Delta\otimes\mathrm{id})(\Phi) + \Phi\otimes\mathrm{id} = (\mathrm{id}\otimes\Delta)(\Phi) + \mathrm{id}\otimes\Phi,$$

which is obviously satisfied since $\Phi = \varphi_1\otimes\varphi_2$.
In general, $2n$ pair-wise commuting derivations φ_i on a commutative algebra $\mathcal{A}$ define a Poisson bracket on $\mathcal{A}$,

$$\{a,b\} = \sum_{i=1}^{n}\left(\varphi_i(a)\cdot\varphi_{i+n}(b) - \varphi_{i+n}(a)\cdot\varphi_i(b)\right),$$

and deformation quantization of the corresponding Poisson algebra $(\mathcal{A},\{\},$ is given by the universal deformation formula

$$m_t = m_0 \circ e^{t\sum_{i=1}^{n}(\varphi_i\otimes\varphi_{i+n} - \varphi_{i+n}\otimes\varphi_i)}.$$

A deformation quantization of a Poisson manifold $(\mathscr{M},\{\},)(see Sec$ - tion 2.7 in Chapter 1) is, by definition, a deformation quantization of the corresponding Poisson algebra of classical observables $(C^\infty(\mathscr{M}),\{\},)$ with the property that the linear maps $m_n, n\geq 1$, are bidifferential operators [28]. The formal power series expansion (3.22) of the $\star$-product is a deformation quantization of the Poisson manifold $(\mathbb{R}^{2n},\{\},)$, where the Poisson bracket corresponding to the canonical symplectic form $\omega = d\boldsymbol{p}\wedge d\boldsymbol{q}$.

Problem 3.

13. Show that $C^\bullet(\mathcal{A},\mathcal{A})$ is a graded Lie algebra with respect to the Gerstenhaber bracket, i.e., that $[,]_G$ satisfies the graded Jacobi identity

$$(-1)^{(m-1)(p-1)}[f,[g,h]] + (-1)^{(n-1)(p-1)}[h,[f,g]] + (-1)^{(m-1)(n-1)}[g,[h,f]] = 0$$

for all $f\in C^m(\mathcal{A},\mathcal{A}), g\in C^n(\mathcal{A},\mathcal{A}), h\in C^p(\mathcal{A},\mathcal{A})$.

Problem 3.

14. Verify that $d_n f = [f,m_0]_G$, where $f\in\mathbb{C}^n(\mathcal{A},\mathcal{A})$ and d_n is the Hochschild differential.

[028] This property ensures that the unit in Poisson algebra is preserved under the deformation.

Problem 3.

15. Show that deformation quantizations associated with Weyl, pq, and ***qp***-quantizations are equivalent. (In fact, all deformation quantizations of the canonical Poisson manifold $(\mathbb{R}^{2n}, \{,\})$*areequivalent.*)

Problem 3.

16. Let $\mathfrak{g}$ be a finite-dimensional Lie algebra with a basis $x_1, ..., x_n$, and let $\mathfrak{g}^*$ be its dual space equipped with the Lie-Poisson bracket $\{,\}$(*seeProblem* 2.20 in Section 2.7 of Chapter 1). For $u \in \mathfrak{g}^*$ and $x = \sum_{i=1}^n \xi^i x_i, y = \sum_{i=1}^n \eta^i x_i \in \mathfrak{g}$ let

$$e^{u\left(\frac{1}{t}\log e^{tx}e^{ty}-x-y\right)} = \sum_{\alpha,\beta} a_{\alpha\beta}(u,t)\xi^\alpha\eta^\beta,$$

where $\xi^\alpha = (\xi^1)^{\alpha_1} ... (\xi^n)^{\alpha_n}, \eta^\beta = (\eta^1)^{\beta_1} ... (\eta^n)^{\beta_n}$, be the formal group law the "Baker-Campbell-Hausdorff series". Show that the product

$$m_t(f_1, f_2) = \sum_{\alpha,\beta} a_{\alpha\beta}(u,t) D^\alpha f_1(u) D^\beta f_2(u), \quad f_1, f_2 \in C^\infty(\mathfrak{g}^*)$$

where for a multi-index $\alpha = (\alpha_1, ..., \alpha_n)$ and $f \in C^\infty(\mathfrak{g}^*), D^\alpha f = \frac{\partial^{\alpha_1+\cdots+\alpha_n} f}{\partial u_1^{\alpha_1} ... \partial u_n^{\alpha_n}}$, gives a deformation quantization of the Poisson manifold $(\mathfrak{g}^*, \{,\})$.

Problem 3.

17. Let $(G, \{\},)$*beaLie* $-$ *Poissongroup, where*$\eta(g) = -r + \mathrm{Ad}^{-1}g \cdot r$ and non-degenerate r satisfies the classical Yang-Baxter equation (see Problems $2.21 - 2.23$ in Section 2.7 of Chapter 1). Using Baker-Campbell-Hausdorff series for the Lie algebra $\tilde{g}$ - the one-dimensional central extension of $\mathfrak{g}$ by the 2 -cocycle c (see Problem 2.23 in Section 2.7 of Chapter 1), show that there exists an element $F \in (U\mathfrak{g} \otimes U\mathfrak{g})[[t]]$ of the form $F = 1 - \frac{1}{2}tr + O(t^2)$, satisfying

$$(\Delta \otimes \mathrm{id})(F)(F \otimes 1) = (\mathrm{id} \otimes \Delta)(F)(1 \otimes F)$$

where Δ is the standard coproduct in $U\mathfrak{g}$.

Problem 3.

18. Let F_L and F_R be the images of F and F^{-1} under the identifications of the universal enveloping algebra $U\mathfrak{g}$ with the algebras of left and rightinvariant differential operators on G (see Problem 2.21 in Section 2.7 of Chapter 1), and let $\mathscr{F} = F_L \circ F_R$. Show that the product $m_t = m_0 \circ \mathscr{F}$ gives a deformation quantization of the Poisson-Lie group $(G, \{,\})$*suchthat*

$$\Delta \circ m_t = (m_t \otimes m_t) \circ \Delta,$$

where Δ is the standard coproduct on functions on $G, \Delta(f)(g_1, g_2) = f(g_1 g_2), f \in C^\infty(G)$. The Hopf algebra $(C^\infty(G), m_t, \Delta, S)$, where S is the standard antipode on $G, S(f)(g) = f(g^{-1})$, is called the quantum group corresponding to the Poisson-Lie group G, and is denoted by $G_q, q = e^t$.

Problem 3.

19. Let $R = \sigma\left(F^{-1}\right) F \in (U\mathfrak{g} \otimes U\mathfrak{g})[[t]]$, where σ is a permutation - an involution of $U\mathfrak{g} \otimes U\mathfrak{g}$, defined by $\sigma(a \otimes b) = b \otimes a, a, b \in U\mathfrak{g}$. Show that $R = 1 - tr + O\left(t^2\right)$ and satisfies the quantum Yang-Baxter equation

$$R_{12}R_{13}R_{23} = R_{23}R_{13}R_{12}$$

(see Problem 2.22 in Section 2.7 in Chapter 1 for notation).

4.3 Integration in Functional Spaces

(maybe later I'll put it to the section of methods)

In the previous chapter we studied the propagator $K\left(\boldsymbol{q}', t; \boldsymbol{q}, 0\right)$ - the integral kernel of the evolution operator $U(t) = e^{-\frac{i}{\hbar}tH}$ - by using its representation by the Feynman path integral. Here we replace the physical time t by the Euclidean time -it, and study the integral kernel of the semigroup $e^{-\frac{1}{\hbar}tH}$ for $t > 0$ by using its representation by the Wiener integral.

4.3.1 1. Gaussian measures

Here we consider the simplest example of Gaussian measures, which are naturally defined for finite-dimensional and infinite-dimensional vector spaces, and are used in many areas of analysis and probability theory. The basic result of the Gaussian integration - the Wick theorem - is the main tool of the perturbation expansion in quantum mechanics and quantum field theory, conveniently expressed through Feynman diagrams.

1.1. Finite-dimensional case.

Let A be a positive-definite, real symmetric $n \times n$ matrix. A basic formula of Gaussian integration is

$$\int_{\mathbb{R}^n} e^{-\frac{1}{2}(A\boldsymbol{q},\boldsymbol{q})} d^n\boldsymbol{q} = \sqrt{\frac{(2\pi)^n}{\det A}} \tag{1.1}$$

(see Lemma 3.1 in Section 3.1 of Chapter 5). The corresponding Gaussian measure associated with the matrix A is a probability measure μ_A on $\mathbb{R}^n$, defined by

$$d\mu_A(\boldsymbol{q}) = \sqrt{\frac{\det A}{(2\pi)^n}} e^{-\frac{1}{2}(A\boldsymbol{q},\boldsymbol{q})} d^n\boldsymbol{q}. \tag{1.2}$$

The measure μ_A is a mean-zero probability measure on $\mathbb{R}^n$ with the covariance $G = A^{-1}$. When $A = I_n$ - the $n \times n$ identity matrix - the corresponding measure is denoted by μ_n.

As follows from Lemma 3.1 in Section 3.1 of Chapter 5,

$$\int_{\mathbb{R}^n} e^{(\boldsymbol{p},\boldsymbol{q})} d\mu_A(\boldsymbol{q}) = e^{\frac{1}{2}(G\boldsymbol{p},\boldsymbol{p})}, \tag{1.3}$$

and by analytic continuation,

$$\int_{\mathbb{R}^n} e^{i(\boldsymbol{p},\boldsymbol{q})} d\mu_A(\boldsymbol{q}) = \lim_{R\to\infty} \int_{\|\boldsymbol{q}\|\le R} e^{i(\boldsymbol{p},\boldsymbol{q})} d\mu_A(\boldsymbol{q}) = e^{-\frac{1}{2}(G\boldsymbol{p},\boldsymbol{p})}. \tag{1.4}$$

The function $(2\pi)^{-\frac{n}{2}} e^{-\frac{1}{2}\langle G\boldsymbol{p},\boldsymbol{p}\rangle}$ is a Fourier transform of the measure μ_A.

Theorem 1.1 (Wick theorem). $\int_{\mathbb{R}^n} (\boldsymbol{v}_1,\boldsymbol{q}) \dots (\boldsymbol{v}_N,\boldsymbol{q})\, d\mu_A(\boldsymbol{q}) = \begin{cases} 0, & N \text{ is odd}, \\ \sum (G\boldsymbol{v}_{i_1},\boldsymbol{v}_{i_2}) \dots \left(G\boldsymbol{v}_{i_{N-1}},\boldsymbol{v}_{i_N}\right), & N \text{ is even}, \end{cases}$, where the sum goes over all possible pairings $(i_1,i_2),\dots,(i_{N-1},i_N)$ - all partitions in pairs of the set $\{1,2,\dots,N\}$.

Proof. Applying to (1.3) the directional derivative along the vector $\boldsymbol{v} \in \mathbb{R}^n$ - the differential operator

$$\partial_{\boldsymbol{v}} = \boldsymbol{v}\frac{\partial}{\partial \boldsymbol{p}} = \sum_{k=1}^{n} v_k \frac{\partial}{\partial p_k}$$

(differentiation under the integral sign is clearly legitimate), we obtain

$$\int_{\mathbb{R}^n} (\boldsymbol{v},\boldsymbol{q}) e^{(\boldsymbol{p},\boldsymbol{q})} d\mu_A(\boldsymbol{q}) = (G\boldsymbol{v},\boldsymbol{p}) e^{\frac{1}{2}(G\boldsymbol{p},\boldsymbol{p})}. \tag{1.5}$$

Setting here $\boldsymbol{p} = 0$ we get

$$\int_{\mathbb{R}^n} (\boldsymbol{v},\boldsymbol{q}) d\mu_A(\boldsymbol{q}) = 0,$$

while applying to (1.5) another $\partial_{\boldsymbol{v}'}$ and setting $\boldsymbol{p} = 0$ afterwards, we obtain

$$\int_{\mathbb{R}^n} (\boldsymbol{v},\boldsymbol{q})\,(\boldsymbol{v}',\boldsymbol{q})\, d\mu_A(\boldsymbol{q}) = (G\boldsymbol{v},\boldsymbol{v}')\,. \tag{1.6}$$

To get the general result, we differentiate (1.3) N times along the vectors $\boldsymbol{v}_1,\dots,\boldsymbol{v}_N$ and set $\boldsymbol{p} = 0$.

Problem 1.1. Let $\boldsymbol{v}_i, \boldsymbol{w}_j \in \mathbb{R}^n$ be such that $(A\boldsymbol{v}_i,\boldsymbol{w}_j) = 0, i,j = 1,\dots,N$, and let F and H be bounded measurable functions on $\mathbb{R}^N$. Show that the functions $f(\boldsymbol{q}) = F\left((\boldsymbol{v}_1,\boldsymbol{q}),\dots,(\boldsymbol{v}_N,\boldsymbol{q})\right)$ and $h(\boldsymbol{q}) = H\left((\boldsymbol{w}_1,\boldsymbol{q}),\dots,(\boldsymbol{w}_N,\boldsymbol{q})\right)$ satisfy

$$\int_{\mathbb{R}^n} f(\boldsymbol{q})h(\boldsymbol{q})d\mu_A(\boldsymbol{q}) = \int_{\mathbb{R}^n} f(\boldsymbol{q})d\mu_A(\boldsymbol{q}) \int_{\mathbb{R}^n} h(\boldsymbol{q})d\mu_A(\boldsymbol{q}).$$

1.2. Infinite-dimensional case.

Let $\mathscr{V} = \mathbb{R}^\infty$ be the Cartesian product of countably many copies of $\mathbb{R}$ equipped with the Tychonoff topology, and let

$$\mathscr{H} = \ell^2(\mathbb{R}) = \left\{ x = \{x_i\}_{i=1}^{\infty} \in \mathscr{V} : \|x\|^2 = \sum_{i=1}^{\infty} x_i^2 < \infty \right\}$$

be the real Hilbert space with the scalar product $(x,y) = \sum_{i=1}^{\infty} x_i y_i$. In particular, the Hilbert space $\mathscr{H}$ contains all elements of finite support: the elements $x \in \mathscr{V}$ such that $x_i = 0$ for sufficiently large i.

The Gaussian measure μ on $\mathscr{V}$ is defined by the direct product of the Gaussian measures μ_1,

$$\mu = \mu_\infty = \mu_1 \times \mu_1 \times \dots \times \mu_1 \times \dots$$

More precisely, the measure μ is defined as follows. Let $\mathscr{C}$ be the set of cylindrical subsets of $\mathscr{V}$: $C \in \mathscr{C}$ if $C = p_n^{-1}(E_1 \times \cdots \times E_n)$ for some n, where $p_n : \mathscr{V} \to \mathbb{R}^n$ is the projection on the Cartesian product of the first n factors, and $E_1, ..., E_n$ are Borel subsets of $\mathbb{R}$. Then we set

$$\mu(C) = \mu_1(E_1) ... \mu_1(E_n),$$

and extend μ to the whole σ-algebra generated by $\mathscr{C}$ by using the Kolmogoroff extension theorem. In particular, if $F(x) = f(x_1, ..., x_n)$, where f is a bounded measurable function on $\mathbb{R}^n$, then

$$\int_{\mathscr{V}} F d\mu = \int_{\mathbb{R}^n} f d\mu_n \tag{1.7}$$

Equivalently, the Gaussian measure μ is characterized by the following property.

Lemma 1.1. The measure μ is a unique probability measure on $\mathscr{V}$ such that for all $v \in \mathscr{V}$ with finite support,

$$\int_{\mathscr{Y}} e^{i(v,x)} d\mu(x) = e^{-\frac{1}{2}\|v\|^2}$$

Proof. The proof immediately follows from (1.4), since measures μ_n are uniquely determined by their Fourier transforms.

Remark. The Gaussian measure μ can be heuristically represented by

$$d\mu = (2\pi)^{-\infty} e^{-\frac{1}{2}\|x\|^2} \prod_{i=1}^{\infty} dx_i$$

Here the "divergent to 0 " product $(2\pi)^{-\infty} e^{-\frac{1}{2}\|x\|^2}$ " compensates the "divergent to ∞ " product $\prod_{i=1}^{\infty} dx_i$.

Now for $\alpha = \{\alpha_i\} \in \mathscr{V}$ let

$$\mathscr{H}_\alpha = \left\{ x \in \mathscr{V} : \sum_{i=1}^{\infty} \alpha_i^2 x_i^2 < \infty \right\}.$$

The following result is a version of Kolmogoroff's celebrated 0-1 law in probability theory.

Proposition 1.1.

$$\mu(\mathscr{H}_\alpha) = \begin{cases} 0 & \text{if } \alpha \notin \mathscr{H} \\ 1 & \text{if } \alpha \in \mathscr{H}. \end{cases}$$

In particular, $\mu(\mathscr{H}) = 0$.

Proof. Let χ_α be the characteristic function of the set $\mathscr{H}_\alpha \subset \mathscr{V}$,

$$\chi_\alpha(x) = \lim_{\varepsilon \to 0} \lim_{n \to \infty} \exp\left\{ -\varepsilon^2 \sum_{i=1}^{n} \alpha_i^2 x_i^2 \right\}.$$

Twice applying the dominated convergence theorem, we get

$$\begin{aligned} \mu(\mathscr{H}_\alpha) &= \int_{\mathscr{Y}} \chi_\alpha d\mu = \lim_{\varepsilon \to 0} \lim_{n \to \infty} \int_{\mathbb{R}^n} \exp\left\{ -\varepsilon^2 \sum_{i=1}^{n} \alpha_i^2 x_i^2 \right\} d\mu_n(x) \\ &= \lim_{\varepsilon \to 0} \lim_{n \to \infty} \prod_{i=1}^{n} \left(1 + \varepsilon^2 \alpha_i^2\right)^{-1/2}, \end{aligned}$$

and the product $\prod_{i=1}^{\infty} (1 + \varepsilon^2 \alpha_i^2)$ is convergent if and only if $\alpha \in \mathscr{H}$.

Remark. For $v \in \mathscr{H}$ let $v^{(n)} = (v_1, ..., v_n, 0, 0, ...)$. It follows from (1.6) that

$$\int_{\mathscr{Y}} \left(v^{(n)}, x\right)^2 d\mu(x) = \left\|v^{(n)}\right\|^2,$$

so that the sequence of functions $F_n(x) = \left(v^{(n)}, x\right), x \in \mathscr{V}$, is a Cauchy sequence in $L^2(\mathscr{V}, d\mu)$, and it converges in L^2 to the function $F(x)$. Abusing notation, we write $F(x) = (v, x) \in L^2(\mathscr{V}, d\mu)$. Thus though $\mu(\mathscr{H}) = 0$, Lemma 1.1 and, consequently, Wick's theorem, hold for $v \in \mathscr{H}$.

Problem 1.2. Prove that there is no probability measure μ on $\mathscr{H}$ such that $\mu(C) = \mu_n(E)$ for every cylindrical subset $C = p_n^{-1}(E)$ of $\mathscr{H}$, where $p_n : \mathscr{H} \to \mathbb{R}^n$ is the natural projection, and E is a Borel subset of $\mathbb{R}^n$. However, show that there exists a finitely-additive, non-negative function ν on cylindrical subsets of $\mathscr{H}$ satisfying this property.

Problem 1.3. Show that the formula

$$\nu\left(\{x \in \mathscr{V} : x_1 \in I_1, ..., x_n \in I_n\}\right) = \prod_{k=1}^{n} \mu_1\left(kI_k\right)$$

where $kI_k = (k\alpha_k, k\beta_k)$ for $I_k = (\alpha_k, \beta_k) \subseteq \mathbb{R}$, defines a probability measure ν on $\mathscr{V}$ such that $\nu(\mathscr{H}) = 1$.

4.3.2 2. Wiener measure and Wiener Integral

2.1. Definition of the Wiener measure.

Here we define the probability measure on the space $\mathscr{C} = C\left([0, \infty), \mathbb{R}^n; 0\right)$ of parametrized continuous paths in $\mathbb{R}^n$ starting at the origin, called the Wiener measure. It is related to the Brownian motion: the diffusion process in $\mathbb{R}^n$ with diffusion coefficient $D > 0$, which is described by the probability density

$$P\left(\boldsymbol{q}', \boldsymbol{q}; t\right) = (4\pi D t)^{-\frac{n}{2}} e^{-\frac{(\boldsymbol{q}-\boldsymbol{q}')^2}{4Dt}} \tag{2.1}$$

that a particle with initial certainty of being at point $\boldsymbol{q} \in \mathbb{R}^n$ is diffused in time t to point $\boldsymbol{q}' \in \mathbb{R}^n$.

It will be convenient to compactify $\mathbb{R}^n$ by adding a point at infinity, $\widehat{\mathbb{R}}^n = \mathbb{R}^n \cup \{\infty\} \simeq S^n$. Let

$$\Omega = \prod_{0 \le t < \infty} \widehat{\mathbb{R}}^n$$

be the Cartesian product of copies of $\widehat{\mathbb{R}}^n$ parametrized by $\mathbb{R}_{\ge 0}$. Equipped with the Tychonoff topology, Ω is a compact topological space - the space of all parametrized paths in $\widehat{\mathbb{R}}^n$. For every partition $\boldsymbol{t}_m = \{0 \le t_1 \le \cdots \le t_m\}$ and every $F \in C(\underbrace{\mathbb{R}^n \times \cdots \times \widehat{\mathbb{R}}^n}_{m})$, define $\varphi \in C(\Omega)$ by

$$\varphi(\gamma) = F\left(\gamma\left(t_1\right), ..., \gamma\left(t_m\right)\right) \quad \text{for all} \quad \gamma \in \Omega$$

We denote by $C_{\text{fin}}(\Omega)$ the subspace of $C(\Omega)$ spanned by the functions φ for all partitions $\boldsymbol{t}_m$ and for all continuous functions F. Define a linear functional l on $C_{\text{fin}}\left(\Omega\right)$ by the following formula:

$$l(\varphi) = \int_{\mathbb{R}^n} ... \int_{\mathbb{R}^n} F\left(\boldsymbol{q}_1, ..., \boldsymbol{q}_m\right) P\left(\boldsymbol{q}_m, \boldsymbol{q}_{m-1}; t_m - t_{m-1}\right) ... \tag{2.2}$$
$$...P\left(\boldsymbol{q}_1, 0; t_1\right) d^n\boldsymbol{q}_1 ... d^n\boldsymbol{q}_m$$

It follows from the semi-group property

$$\int_{\mathbb{R}^n} P(\boldsymbol{q}', \boldsymbol{q}_1; t' - t_1) P(\boldsymbol{q}_1, \boldsymbol{q}; t_1 - t) d^n \boldsymbol{q}_1 = P(\boldsymbol{q}', \boldsymbol{q}; t' - t)$$

(also called Kolmogoroff's equation in probability theory) that the functional l is well defined. The functional l is positive: $l(\varphi) \geq 0$ for $\varphi \geq 0$, satisfies $l(1) = 1$, and

$$|l(\varphi)| \leq \|\varphi\|_\infty = \sup_{\gamma \in \Omega} |\varphi(\gamma)|.$$

The subspace $C_{\text{fin}}(\Omega)$ separates points in Ω and $1 \in C_{\text{fin}}(\Omega)$, so that by the Stone-Weierstrass theorem $C_{\text{fin}}(\Omega)$ is dense in $C(\Omega)$. Now the functional l has a unique extension to a continuous positive linear functional on $C(\Omega)$ with norm 1, and by the Riesz-Markoff theorem, there exists a unique regular Borel measure μ_W on Ω with $\mu_W(\Omega) = 1$ such that

$$l(\varphi) = \int_\Omega \varphi d\mu_W$$

The measure μ_W is called the Wiener measure. The integral over the Wiener measure is called the Wiener integral.

Remark. The Riesz-Markoff theorem provides a natural way of defining measures in various problems of functional analysis. In general, it ensures the existence of a Baire measure — a measure defined on the σ-algebra of Baire sets. However, for compact spaces a Baire measure has a unique extension to a regular Borel measure - a measure defined on the σ-algebra generated by all open subsets. A Borel measure μ is regular, if for every Borel set $E \subseteq \Omega$,

$$\mu(E) = \begin{cases} \inf \mu(U), & E \subseteq U, U \text{ is open,} \\ \sup \mu(K), & K \subseteq E, K \text{ is compact and Borel.} \end{cases}$$

The space Ω is "so large" that its σ-algebras of Baire and Borel sets are different.

Proposition 2.1. The Wiener measure μ_W is supported on continuous paths starting at the origin, i.e., $\mu_W(\mathscr{C}) = 1$.

Replacing the probability density $P(\boldsymbol{q}_1, 0; t_1)$ by $P(\boldsymbol{q}_1, \boldsymbol{q}_0; t_1)$ in definition (2.2), for a fixed $\boldsymbol{q}_0 \in \mathbb{R}^n$ we obtain a Wiener measure $\mu_{\boldsymbol{q}_0}$, which is supported on the space $\mathscr{C}_{\boldsymbol{q}_0} = C([0, \infty), \mathbb{R}^n; \boldsymbol{q}_0)$ of continuous paths in $\mathbb{R}^n$ that start at $\boldsymbol{q}_0$.

Remark. The support of the Wiener measure μ_W can be characterized more precisely as follows. For $0 < \alpha \leq 1$ let Ω_α be the subspace of Ω of Hlder continuous paths of order α:

$$\Omega_\alpha = \left\{ \gamma \in \Omega : \sup_{t, t' \geq 0} \frac{\|\gamma(t) - \gamma(t')\|}{|t - t'|^\alpha} < \infty \right\}.$$

Then

$$\mu_W(\Omega_\alpha) = \begin{cases} 1, & \text{if } 0 < \alpha < \frac{1}{2} \\ 0, & \text{if } \frac{1}{2} \leq \alpha \leq 1 \end{cases}$$

Remark. It seems natural to define Wiener measure by the following construction. Set for simplicity $n = 1$, and for every partition $\boldsymbol{t}_m = \{0 \leq t_1 \leq \cdots \leq t_m\}$ and intervals $(\alpha_1, \beta_1), ..., (\alpha_m, \beta_m)$, define the measure of a cylindrical set

$$C_t = \{\gamma \in \Omega : \alpha_1 < \gamma(t_1) < \beta_1, ..., \alpha_m < \gamma(t_m) < \beta_m\}$$

by the formula

$$\mu\left(C_{\boldsymbol{t}}\right)=\int_{\alpha_1}^{\beta_1}...\int_{\alpha_m}^{\beta_m}P\left(q_m,q_{m-1};t_m-t_{m-1}\right)...P\left(q_1,0;t_1\right)dq_1...dq_m \tag{2.3}$$

By the Kolmogoroff extension theorem and the semi-group property, μ extends to a measure on the σ-algebra generated by the cylindrical subsets of Ω, which we continue to denote by μ. However, the set $\mathscr{C}$ of continuous paths starting at 0 turns out to be non-measurable! Specifically, one can show that

$$\mu_*(\mathscr{C})=0 \quad \text{and} \quad \mu^*(\mathscr{C})=1$$

where $\mu_*(E)$ and $\mu^*(E)$ denote, respectively, the inner and outer measures of the subset $E\subseteq\Omega$. To remedy this situation, one should from the beginning define cylindrical sets C_t as consisting of continuous paths only, and define $\mu\left(C_{\boldsymbol{t}}\right)$ by the same formula as above. Then the measure μ extends to a σ algebra generated by cylindrical subsets of $\mathscr{C}$, and coincides with the Wiener measure μ_W.

Remark. The same formula (2.3) can be used to define the Wiener measure on the space $C([0,\pi],\mathbb{R};0)$ of continuous functions on the interval $[0,\pi]$ which vanish at $t=0$; in this case $\boldsymbol{t}_m$ is a partition of $[0,\pi]$. This is the classical definition of the Wiener measure given by Wiener himself.

The following result will be used for representing the integral kernel of the one-parameter semigroup $e^{-\frac{1}{\hbar}tH}$ for $t>0$ by the Wiener integral.

Proposition 2.2. Let the real-valued function $V\in C\left(\mathbb{R}^n\right)$ be bounded below. Then for every $t\geq 0$ the function $\mathcal{F}_t:\mathscr{C}\to\mathbb{R}$, defined by

$$\mathcal{F}_t(\gamma)=e^{-\int_0^t V(\gamma(\tau))d\tau}$$

is integrable with respect to the Wiener measure, and

$$\int_{\mathscr{C}}\mathcal{F}_t d\mu_W=\lim_{N\to\infty}\int_{\mathbb{R}^n}...\int_{\mathbb{R}^n}\exp\left\{-\sum_{k=1}^{N}V\left(\boldsymbol{q}_k\right)\Delta t\right\}P\left(\boldsymbol{q}_N,\boldsymbol{q}_{N-1};\Delta t\right)...$$
$$...P\left(\boldsymbol{q}_1,0;\Delta t\right)d^n\boldsymbol{q}_1...d^n\boldsymbol{q}_N,\quad \Delta t=\frac{t}{N}$$

Proof. For $\gamma\in\mathscr{C}$,

$$\int_0^t V(\gamma(\tau))d\tau=\lim_{N\to\infty}\sum_{k=1}^{N}V\left(\gamma\left(t_k\right)\right)\Delta t$$

where $t_k=k\Delta t$. Since by definition every function $\sum_{k=1}^{N}V\left(\gamma\left(t_k\right)\right)\Delta t$ is measurable with respect to the Wiener measure on $\mathscr{C}$, the function $\mathcal{F}_t$ is measurable as a point-wise limit of a sequence of measurable functions. The function $\mathcal{F}_t$ is bounded and, therefore, is integrable on $\mathscr{C}$ with respect to the Wiener measure. Finally, by the dominated convergence theorem,

$$\int_{\mathscr{C}}\mathcal{F}_t d\mu_W=\lim_{N\to\infty}\int_{\mathscr{C}}\exp\left\{-\sum_{k=1}^{N}V\left(\gamma\left(t_k\right)\right)\Delta t\right\}d\mu_W(\gamma)$$

and the result follows from (2.2).

Remark. Note the limit in Proposition 2.2 exists because the function $\mathcal{F}_t$ is integrable, and not the other way around. This is similar to an elementary calculus argument that the limit

$$\lim_{n\to\infty}\left(1+\frac{1}{2}+\cdots+\frac{1}{n}-\log n\right)$$

exists because the integral

$$\int_0^1 \left(\frac{1}{x} - \left[\frac{1}{x}\right]\right) dx$$

is convergent. Here $[x]$ stands for the largest integer not greater than x.

Problem 2.1. Prove all statements about the support of Wiener measure.

Problem 2.2. Construct the Wiener measure by defining it on the cylindrical subsets of $\mathscr{C}$ by formula (2.3).

Problem 2.3. Prove that the Wiener measure μ_W on $C([0,\pi],\mathbb{R};0)$ for $D = \frac{1}{4}$ actually coincides with the measure ν defined in Problem 1.3. (Hint: Show that the mapping $\gamma(t) \mapsto \gamma(t)-\gamma(0)$ establishes the isomorphism between the space of $\hat{C}([0,\pi],\mathbb{R})$ of functions orthogonal to 1 and $C([0,\pi],\mathbb{R};0)$, and use the Fourier sine coefficients for the embedding $\hat{C}([0,\pi],\mathbb{R}) \hookrightarrow \mathscr{V}$.)

2.2. Conditional Wiener measure and Feynman-Kac formula. Let

$$\Omega_{\boldsymbol{q},\boldsymbol{q}'} = \left\{\boldsymbol{\gamma} \in \prod_{t\le\tau\le t'} \widehat{\mathbb{R}}^n : \boldsymbol{\gamma}(t) = \boldsymbol{q}, \boldsymbol{\gamma}(t') = \boldsymbol{q}'\right\}$$

be the space of all parametrized paths in $\widehat{\mathbb{R}}^n$ which start at $\boldsymbol{q} \in \mathbb{R}^n$ at time t and end at $\boldsymbol{q}' \in \mathbb{R}^n$ at t', and let $\mathscr{C}_{\boldsymbol{q},\boldsymbol{q}'}$ be the corresponding subspace of continuous paths. The conditional Wiener measure $\mu_{\boldsymbol{q},\boldsymbol{q}'}$ on $\Omega_{\boldsymbol{q},\boldsymbol{q}'}$ is defined
similarly. We replace a positive linear functional l on $C(\Omega)$ by a positive linear functional $l_{\boldsymbol{q},\boldsymbol{q}'}$ on $C(\Omega_{\boldsymbol{q},\boldsymbol{q}'})$, which for $\varphi \in C_{\text{fin}}(\Omega_{\boldsymbol{q},\boldsymbol{q}'})$ is defined by

$$l_{\boldsymbol{q},\boldsymbol{q}'}(\varphi) = \int_{\mathbb{R}^n} ... \int_{\mathbb{R}^n} F(\boldsymbol{q}_1,...,\boldsymbol{q}_m) P(\boldsymbol{q}',\boldsymbol{q}_m;t'-t_m) ...$$
$$...P(\boldsymbol{q}_1,\boldsymbol{q};t_1-t)\, d^n\boldsymbol{q}_1...d^n\boldsymbol{q}_m$$

where $t \le t_1 \le \cdots \le t_m \le t'$ and $\varphi(\gamma) = F(\gamma(t_1),...,\gamma(t_m))$. Then

$$l_{\boldsymbol{q},\boldsymbol{q}'}(\varphi) = \int_{\Omega_{\boldsymbol{q},\boldsymbol{q}'}} \varphi d\mu_{\boldsymbol{q},\boldsymbol{q}'}$$

As in the case of the Wiener measure μ_W, the conditional Wiener measure $\mu_{\boldsymbol{q},\boldsymbol{q}'}$ is supported on continuous paths and

$$\mu_{\boldsymbol{q},\boldsymbol{q}'}(\mathscr{C}_{\boldsymbol{q},\boldsymbol{q}'}) = P(\boldsymbol{q}',\boldsymbol{q};t'-t)$$

Let

$$H = H_0 + V = \frac{\boldsymbol{P}^2}{2m} + V(\boldsymbol{Q})$$

be the Schrodinger operator on $L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ with continuous, real-valued and bounded below potential $V(\boldsymbol{q})$. Denote by $L_\hbar(\boldsymbol{q}',t';\boldsymbol{q},t), t' > t$, the heat kernel - the integral kernel of the diffusion operator $e^{-\frac{t'-t}{\hbar}H}$. Here is the main result of this section.

Theorem 2.1 (Feynman-Kac formula).

$$L_\hbar(\boldsymbol{q}',t';\boldsymbol{q},t) = \int_{\mathscr{C}_{\boldsymbol{q},\boldsymbol{q}'}} e^{-\frac{1}{\hbar}\int_t^{t'} V(\gamma(\tau))d\tau} d\mu_{\boldsymbol{q},\boldsymbol{q}'}(\boldsymbol{\gamma})$$

where $\mu_{\boldsymbol{q},q'}$ is the conditional Wiener measure.

Proof. We have by the Lie-Kato-Trotter product formula

$$e^{-\frac{1}{\hbar}TH} = \lim_{N\to\infty}\left(e^{-\frac{\Delta t}{\hbar}H_0}e^{-\frac{\Delta t}{\hbar}V}\right)^N, \quad \Delta t = \frac{T}{N}$$

where $T = t'-t$. Let $L_\hbar^{(N)}(\boldsymbol{q}', t'; \boldsymbol{q}, t)$ be the integral kernel of the operator $\left(e^{-\frac{\Delta t}{\hbar}H_0}e^{-\frac{\Delta t}{\hbar}V}\right)^N$. Computing it as in Section 1.3 of Chapter 5, and using the definition of the conditional Wiener measure we obtain

$$L_\hbar^{(N)}(\boldsymbol{q}', t'; \boldsymbol{q}, t) = \int_{\mathscr{C}_{\boldsymbol{q},\boldsymbol{q}'}} \exp\left\{-\frac{1}{\hbar}\sum_{k=1}^{N} v\left(\gamma\left(t_k\right)\right)\Delta t\right\} d\mu_{\boldsymbol{q},\boldsymbol{q}'}(\gamma)$$

Evaluating the limit $N \to \infty$ by the dominated convergence theorem completes the proof.
Using the conditional Wiener measure it is easy to define a measure μ_W^{loop} on the space

$$\mathcal{L} = \left\{\gamma \in \prod_{t\le\tau\le t'} \widehat{\mathbb{R}}^n : \gamma(t) = \gamma\left(t'\right)\right\}$$

of free parametrized loops in $\widehat{\mathbb{R}}^n$. Namely, the space $\mathcal{L}$ is a disjoint union over $\boldsymbol{q} \in \widehat{\mathbb{R}}^n$ of the spaces $\Omega_{\boldsymbol{q},\boldsymbol{q}}$ of the parametrized loops based at $\boldsymbol{q} \in \widehat{\mathbb{R}}^n$. By definition, a function $\varphi : \mathcal{L} \to \mathbb{C}$ is called integrable, if its restrictions $\varphi|_{\Omega_{q,q}}$ are measurable with respect to $\mu_{\boldsymbol{q},\boldsymbol{q}}$ for all $\boldsymbol{q} \in \mathbb{R}^n$, and if the function $\int_{\Omega_{q,\boldsymbol{q}}} \varphi d\mu_{\boldsymbol{q},\boldsymbol{q}} : \mathbb{R}^n \to \mathbb{C}$ is Lebesgue integrable on $\mathbb{R}^n$. Then

$$\int_{\mathcal{L}} \varphi d\mu_W^{\text{loop}} = \int_{\mathbb{R}^n}\int_{\Omega_{\boldsymbol{q},\boldsymbol{q}}} \varphi d\mu_{\boldsymbol{q},\boldsymbol{q}} d^n\boldsymbol{q} \tag{2.4}$$

Suppose that the Schrodinger operator $H = H_0 + V$ with continuous, real-valued, and bounded below potential $V(\boldsymbol{q})$ has a pure point spectrum, and that $e^{-\frac{T}{\hbar}H}$ is of trace class [1]. The following result is a useful corollary of the Feynman-Kac formula.

Corollary 2.2.

$$\operatorname{Tr} e^{-\frac{T}{\hbar}H} = \int_{\mathcal{L}} e^{-\frac{1}{\hbar}\int_0^T V(\gamma(t))dt} d\mu_W^{\text{loop}}(\gamma)$$

Proof. The heat kernel $L_\hbar(\boldsymbol{q}', T; \boldsymbol{q}, 0)$ - the integral kernel of the trace class operator $e^{-\frac{T}{\hbar}H}$ - is a continuous function of $\boldsymbol{q}$ and $\boldsymbol{q}'$, so that by the theorem [2] that "the operator trace equals the matrix trace", used in Sections $5.1 - 5.2$ of Chapter 5, we get

$$\operatorname{Tr} e^{-\frac{T}{\hbar}H} = \int_{\mathbb{R}^n} L_\hbar(\boldsymbol{q}, T; \boldsymbol{q}, 0) d^n\boldsymbol{q}$$

The result now follows from the Feynman-Kac formula and equation (2.4).
Remark. The Wiener measure on the loop space

$$\mathcal{L} = \{\gamma \in C([0,T], \mathbb{R}) : \gamma(0) = \gamma(T)\}$$

in terms of the Fourier coefficients

$$\gamma(t) = \sum_{n=-\infty}^{\infty} c_n e^{\frac{2\pi i n t}{T}}, \quad \bar{c}_n = c_{-n}$$

can be expressed as follows:

$$d\mu_W^{\text{loop}} = \sqrt{\frac{m}{2\pi\hbar T}} dc_0 \prod_{n=1}^{\infty} \left(\frac{m}{\pi\hbar T}\right) (2\pi n)^2 e^{-\frac{m}{\hbar T}(2\pi n)^2 |c_n|^2} d^2 c_n \tag{2.5}$$

In particular,

$$\int_{\mathcal{L}} f(\gamma) d\mu_W^{\text{loop}}(\gamma) = \sqrt{\frac{m}{2\pi\hbar T}} \int_{-\infty}^{\infty} \left(\int_{\mathcal{L}_0} f(x, \gamma_0)\, d\mu_W^{\text{loop}}(\gamma_0) \right) dx \tag{2.6}$$

Here $\mathcal{L}_0$ is the space of loops γ_0 with $c_0 = 0$, and $\mathcal{L} = \mathbb{R} \times \mathcal{L}_0$ according to the decomposition $\gamma = x + \gamma_0$, where $\int_0^T \gamma_0(t) dt = 0$ so that $x = c_0(\gamma)$.

Problem 2.4. Deduce from the Feynman-Kac formula that for every $\psi \in L^2(\mathbb{R}^n)$,

$$\left(e^{-\frac{1}{\hbar}T(H_0+V)}\psi\right)(\boldsymbol{q}) = \int_{\mathscr{C}_{\boldsymbol{q}}} \psi(\gamma(t)) e^{-\frac{1}{\hbar}\int_0^T V(\gamma(t))dt} d\mu_{\boldsymbol{q}}(\gamma).$$

Problem 2.5. Prove formula (2.5) and deduce (2.6) from it. (Hint: Use Problem 2.3.)

2.3. Relation between Wiener and Feynman integrals. It is very instructive to compare Feynman and Wiener integrals. Heuristically, the conditional Wiener measure can be written as

$$\mathscr{D}\boldsymbol{q}_W = e^{-\frac{m}{2\hbar}\int_t^{t'} \dot{\boldsymbol{q}}^2 d\tau} \mathscr{D}_\hbar \boldsymbol{q} \tag{2.7}$$

where

$$\mathscr{D}_\hbar \boldsymbol{q} = \lim_{N\to\infty} \left(\frac{m}{2\pi\hbar\Delta t}\right)^{\frac{N}{2}} \prod_{k=1}^{N-1} d^n \boldsymbol{q}_k. \tag{2.8}$$

Of course, neither the "measure" $\mathscr{D}_\hbar \boldsymbol{q}$ exists: the infinite product (2.8) is divergent, nor the trajectory $\gamma = \boldsymbol{q}(\tau)$ is, in general, differentiable: the integral $\int_t^{t'} \dot{\boldsymbol{q}}^2 d\tau$ is divergent. However, due to the presence of a negative sign in the exponential, we have the indeterminate form "infinity over infinity", and the resulting expression (2.7) can be given a precise meaning as the Wiener measure. The corresponding "measure" for the Feynman path integral is obtained by replacing $\hbar$ by $i\hbar$ in (2.7)-(2.8), and the exponential factor no longer compensates for the divergence of $\mathscr{D}_{i\hbar}\boldsymbol{q}$, since it is a complex number of modulus 1 for a differentiable trajectory, and has no meaning for a non-differentiable one.

However, as we have seen in Sections 1.3-1.4 of Chapter 5, the Feynman path integral allows us to represent the propagator of a quantum particle in a profound way, which shows a deep relation between quantum and classical mechanics. Namely,

$$K_\hbar(\boldsymbol{q}', t'; \boldsymbol{q}, t) = \int_{\substack{\boldsymbol{q}(t')=q' \\ \boldsymbol{q}(t)=\boldsymbol{q}}} e^{\frac{i}{\hbar}S(\gamma)} \mathscr{D}_{i\hbar}\boldsymbol{q},$$

where $S(\gamma) = \int_t^{t'} L(\boldsymbol{q}, \dot{\boldsymbol{q}}) d\tau$ is the action functional evaluated on a trajectory $\boldsymbol{\gamma} = \boldsymbol{q}(\tau)$, and $L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \frac{1}{2}m\dot{\boldsymbol{q}}^2 - V(\boldsymbol{q})$ is the corresponding Lagrangian function. One also can formally rewrite the Wiener integral for the integral kernel $L_\hbar(\boldsymbol{q}', t'; \boldsymbol{q}, t)$ - the Feynman-Kac formula - in a similar form,

$$L_\hbar(\boldsymbol{q}', t'; \boldsymbol{q}, t) = \int_{\substack{\boldsymbol{q}(t')=q' \\ \boldsymbol{q}(t)=\boldsymbol{q}}} e^{-\frac{1}{\hbar}\int_t^{t'} E(\boldsymbol{q},\boldsymbol{q})d\tau} \mathscr{D}_\hbar \boldsymbol{q}$$

[01] This is the case when $V(\boldsymbol{q}) \to \infty$ as $\boldsymbol{q} \to \infty$ "fast enough", i.e., $V(q) \geq C\|\boldsymbol{q}\|^2$.

[2] See Section 7 of Chapter 5 for the reference.

where $E(\boldsymbol{q},\dot{\boldsymbol{q}}) = \frac{1}{2}m\dot{\boldsymbol{q}}^2 + V(\boldsymbol{q})$ is the energy function. However, in this representation we no longer see the presence of the corresponding action functional, and connection with the classical mechanics is lost.

The precise relation between Wiener and Feynman integrals for a quantum particle is the following. As in the case of the Feynman-Kac formula, suppose that the real-valued potential $V(\boldsymbol{q}) \in C(\mathbb{R}^n)$ is bounded below. Using the Lie-Kato-Trotter formula, it is easy to show that the heat kernel $L_\hbar(\boldsymbol{q}',t';\boldsymbol{q},t)$, defined for $\hbar > 0$, admits an analytic continuation into the half-plane $\operatorname{Re}\hbar > 0$. Then

$$K_\hbar(\boldsymbol{q}',t';\boldsymbol{q},t) = \lim_{\varepsilon\to 0^+} L_{i\hbar+\varepsilon}(\boldsymbol{q}',t';\boldsymbol{q},t) \tag{2.9}$$

Remark. Let f be a smooth bounded function on $\mathbb{R}$ such that $f'(x) = O(|x|^{-1})$ as $|x| \to \infty$. The Gaussian integral $\int_{-\infty}^{\infty} f(x)e^{-x^2}dx$ is absolutely convergent, whereas the integral $\int_{-\infty}^{\infty} f(x)e^{ix^2}dx$ is only conditionally convergent. The formula

$$\int_{-\infty}^{\infty} f(x)e^{ix^2}dx = \lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} f(x)e^{(i-\varepsilon)x^2}dx$$

interprets it as the limit $\varepsilon \to 0$ of an integral with respect to the complexvalued Gaussian measure $e^{(i-\varepsilon)x^2}dx$. It is tempting to extend this interpretation to Wiener integrals, and for a complex diffusion coefficient D with $\operatorname{Re} D > 0$ to define a complex-valued Wiener measure by the same formula (2.2). However, a theorem of Cameron states that the linear functional l, defined by an analog of (2.2) for $\operatorname{Re} D > 0$, is no longer bounded on $C_{\text{fin}}(\Omega)$, so that this approach does not work.

Problem 2.6. Let l be the functional on $C_{\text{fin}}(\Omega)$ defined by (2.2) where $P(\boldsymbol{q}',\boldsymbol{q},t)$ is given by (2.1) with $\operatorname{Re} D \geq 0$.
(i) Prove that when $\operatorname{Re} D = 0$,

$$\sup_{t\geq 0, F\in C(\hat{\mathbb{R}})}\{|l(\varphi)| : \|\varphi\|_\infty = 1, \varphi(\gamma) = F(\gamma(t))\} = \infty.$$

(ii) Prove that when $\operatorname{Re} D > 0$,

$$\sup_{\boldsymbol{t}_m, F\in C(\mathbb{R}^m)}\{|l(\varphi)| : \|\varphi\|_\infty = 1, \varphi(\gamma) = F(\gamma(t_1),...,\gamma(t_m))\} = \left(\frac{|D|}{\operatorname{Re} D}\right)^m.$$

4.3.3 3. Gaussian Wiener Integrals

In Section 4 of Chapter 5 we evaluated Gaussian Feynman integrals in terms of the regularized determinants of corresponding differential operators. Here we consider the same problem for Gaussian Wiener integrals.

3.1. Dirichlet boundary conditions.

Let

$$A = -D^2 + u(t), \quad D = \frac{d}{dt},$$

where $u \in C^1([0,T])$, be the Sturm-Liouville operator on the interval $[0,T]$ with Dirichlet boundary conditions. The following result is fundamental.

Theorem 3.1. Suppose that $u(t) \geq 0$. Then

$$\int_{\mathscr{C}_{0,0}} e^{-\frac{m}{2\hbar}\int_0^T u(t)y^2(t)dt} d\mu_{0,0}(y) = \sqrt{\frac{m}{\pi\hbar \det A}}$$

Proof. Using Proposition 2.2 and finite-dimensional Gaussian integration formula (1.1), we get

$$\int_{\mathscr{C}_{0,0}} e^{-\frac{m}{2\hbar}\int_0^T u(t)y^2(t)dt} d\mu_{0,0}(y) = \lim_{n\to\infty} \left(\frac{m}{2\pi\hbar\Delta t}\right)^{\frac{n}{2}} \int \ldots \int$$
$$\exp\left\{-\frac{m}{2\hbar\Delta t}\sum_{k=0}^{n-1}\left(\left(y_{k+1}-y_k\right)^2 + u\left(t_k\right)\left(\Delta t\right)^2 y_k^2\right)\right\}\prod_{k=1}^{n-1} dy_k$$
$$= \lim_{n\to\infty}\sqrt{\frac{m}{2\pi\hbar\Delta t \det A_{n-1}}}$$

(cf. the proof of Proposition 3.1 in Section 3.2 of Chapter 5). Here $y_0 = y_n = 0, t_k = k\Delta t, \Delta t = \frac{T}{n}$, and

$$A_{n-1} = \begin{pmatrix} a_1 & -1 & 0 & \cdots & 0 & 0 \\ -1 & a_2 & -1 & \cdots & 0 & 0 \\ 0 & -1 & a_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & a_{n-2} & -1 \\ 0 & 0 & 0 & \cdots & -1 & a_{n-1} \end{pmatrix}$$

where $a_k = 2 + u\left(t_k\right)\left(\Delta t\right)^2, k = 1, \ldots, n-1$. Let $y_k^{(n)}$ be Δt times the principal minor of order $k-1$ of the matrix A_{n-1} corresponding to its upper-left corner, so that $y_n^{(n)} = \Delta t \det A_{n-1}$. The sequence $y_k^{(n)}$ satisfies the initial conditions

$$y_2^{(n)} = 2\Delta t + O\left(\left(\Delta t\right)^3\right), \quad y_3^{(n)} = 3\Delta t + O\left(\left(\Delta t\right)^3\right)$$

and expanding the order k determinant $y_{k+1}^{(n)}$ with respect to the last row, we obtain the recurrence relation

$$y_{k+1}^{(n)} + y_{k-1}^{(n)} - 2y_k^{(n)} = u\left(t_k\right)\left(\Delta t\right)^2 y_k^{(n)}, \quad k = 3, \ldots, n-1$$

Since

$$\lim_{k,n\to\infty} u\left(t_k\right) = u(t) \quad \text{when} \quad \lim_{k,n\to\infty} t_k = t$$

it follows from the method of finite-differences for solving initial value problem for ordinary differential equations that

$$\lim_{k,n\to\infty} y_k^{(n)} = y(t)$$

where $y(t)$ is the solution of the differential equation

$$-y'' + u(t)y = 0$$

with the initial conditions

$$y(0) = \lim_{n\to\infty} y_2^{(n)} = 0, \quad y'(0) = \lim_{n\to\infty} \frac{y_3^{(n)} - y_2^{(n)}}{\Delta t} = 1$$

Using Theorem 5.1 in Section 5.1 of Chapter 5, we finally obtain

$$\lim_{n\to\infty} \Delta t \det A_{n-1} = \lim_{n\to\infty} y_n^{(n)} = y(T) = \frac{1}{2}\det{}' A$$

Remark. The same computation also works for Feynman path integrals, and gives a rigorous proof of the formula

$$\int_{\left\{\begin{array}{l} y(T)=0 \\ y(0)=0 \end{array}\right\}} e^{\frac{im}{2\hbar}\int_0^T \left(\dot{y}^2 - u(t)y^2\right)dt} \mathscr{D}y = \sqrt{\frac{m}{\pi i\hbar \det A}}$$

where $A = -D^2 - u(t)$ is a positive-definite operator (see Section 6.1 of Chapter 5). In particular, the coefficient $c_{m,\hbar}$ from Section 4 of Chapter 5 is indeed equal to $\sqrt{\frac{m}{\pi i\hbar}}$.

3.2. Periodic boundary conditions. Let $A = -D^2 + u(t)$, where $u \in C^1([0,T])$, be the Sturm-Liouville operator on the interval $[0,T]$ with periodic boundary conditions. Here we prove the following analog of Theorem 3.1.

Theorem 3.2. Suppose that $u(t) > 0$. Then

$$\int_{\mathcal{L}} e^{-\frac{m}{2\hbar}\int_0^T u(t)y^2(t)dt} d\mu_W^{\text{loop}}(y) = \frac{1}{\sqrt{\det A}}$$

where $\mathcal{L}$ is the space of free loops in $\mathbb{R}$ parametrized by the interval $[0,T]$.

Proof. As in the proof of Theorem 3.1, we have

$$\int_{\mathcal{L}} e^{-\frac{m}{2\hbar}\int_0^T u(t)y^2(t)dt} d\mu_W^{\text{loop}}(y) = \lim_{n\to\infty} \left(\frac{m}{2\pi\hbar\Delta t}\right)^{\frac{n}{2}} \int\cdots\int$$
$$\exp\left\{-\frac{m}{2\hbar\Delta t}\sum_{k=0}^{n-1}\left(\left(y_{k+1}-y_k\right)^2 + u\left(t_k\right)\left(\Delta t\right)^2 y_k^2\right)\right\}\prod_{k=1}^{n} dy_k$$
$$= \lim_{n\to\infty} \frac{1}{\sqrt{\det A_n}}$$

Here $y_0 = y_n$ and A_n is the following $n \times n$ matrix:

$$A_n = \begin{pmatrix} a_0 & -1 & 0 & \cdots & 0 & -1 \\ -1 & a_1 & -1 & \cdots & 0 & 0 \\ 0 & -1 & a_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & a_{n-2} & -1 \\ -1 & 0 & 0 & \cdots & -1 & a_{n-1} \end{pmatrix}$$

where $a_k = 2 + u\left(t_k\right)\left(\Delta t\right)^2, k = 0, 1, ..., n-1$. We compute $\det A_n$ by the following elegant argument. First, note that the real λ is an eigenvalue of A_n if only if the difference equation

$$-\left(y_{k+1} + y_{k-1} - 2y_k\right) + u\left(t_k\right)\left(\Delta t\right)^2 y_k = \lambda y_k, \quad k = 0, ..., n-1 \tag{3.1}$$

with initial conditions y_{-1} and y_0 has a "periodic solution" - a solution $\{y_k\}_{k=1}^n$ satisfying $y_{n-1} = y_{-1}$ and $y_n = y_0$. For given λ denote by $v_k^{(1)}(\lambda)$ and $v_k^{(2)}(\lambda)$ solutions of (3.1) with the corresponding initial conditions $v_{-1}^{(1)}(\lambda) = 1, v_0^{(1)}(\lambda) = 0$ and $v_{-1}^{(2)}(\lambda) = 0, v_0^{(2)}(\lambda) = 1$, and put

$$T_n(\lambda) = \begin{pmatrix} v_{n-1}^{(1)}(\lambda) & v_{n-1}^{(2)}(\lambda) \\ v_n^{(1)}(\lambda) & v_n^{(2)}(\lambda) \end{pmatrix}$$

It is easy to show that the discrete analog of the Wronskian $v_{k-1}^{(1)}(\lambda)v_k^{(2)}(\lambda)$ - $v_k^{(1)}(\lambda)v_{k-1}^{(2)}(\lambda)$ does not depend on k, so that $\det T_n(\lambda) = 1$. Since every solution y_k of the initial value problem for (3.1) is a linear combination of the solutions $v_k^{(1)}(\lambda)$ and $v_k^{(2)}(\lambda)$, we have

$$\begin{pmatrix} y_{n-1} \\ y_n \end{pmatrix} = T_n(\lambda) \begin{pmatrix} y_{-1} \\ y_0 \end{pmatrix}$$

From here we conclude that λ is an eigenvalue of the matrix A_n if and only if $\det(T_n(\lambda) - I_2) = 0$, and the multiplicity of λ is the multiplicity of a root of this algebraic equation. Since

$$v_{n-1}^{(1)}(\lambda) = O\left(\lambda^{n-1}\right), \quad v_n^{(2)}(\lambda) = (-\lambda)^n + O\left(\lambda^{n-1}\right) \quad \text{as} \quad \lambda \to \infty$$

we obtain

$$\det(A_n - \lambda I_n) = -\det(T_n(\lambda) - I_2) = v_{n-1}^{(1)}(\lambda) + v_n^{(2)}(\lambda) - 2.$$

It remains to compute $\lim_{n\to\infty} \det(A_n - \lambda I_n)$. Denote by $y_k^{(1)}(\lambda)$ and $y_k^{(2)}(\lambda)$, correspondingly, two solutions of the difference equation (3.1) with the initial conditions $y_{-1}^{(1)}(\lambda) = y_0^{(1)}(\lambda) = 1$ and $y_{-1}^{(2)}(\lambda) = 0, y_0^{(2)}(\lambda) = \Delta t$. We have

$$v_k^{(1)}(\lambda) = y_k^{(1)}(\lambda) - \frac{1}{\Delta t} y_k^{(2)}(\lambda) \quad \text{and} \quad v_k^{(2)}(\lambda) = \frac{1}{\Delta t} y_k^{(2)}(\lambda)$$

so that

$$\det(A_n - \lambda I_n) = y_{n-1}^{(1)}(\lambda) + \frac{y_n^{(2)}(\lambda) - y_{n-1}^{(2)}(\lambda)}{\Delta t} - 2 \tag{3.2}$$

Now it follows from the method of finite differences that

$$\lim_{k,n\to\infty} y_k^{(1)}(\lambda) = y_1(t,\lambda), \quad \lim_{k,n\to\infty} y_k^{(2)}(\lambda) = y_2(t,\lambda) \tag{3.3}$$

as $\lim_{k,n\to\infty} t_k = t$, where $y_{1,2}(t,\lambda)$ are two solutions of the differential equation

$$-y'' + u(t)y = \lambda y$$

with the initial conditions $y_1(0,\lambda) = 1, y_1'(0,\lambda) = 0$ and $y_2(0,\lambda) = 0$, $y_2'(0,\lambda) = 1$. Using (3.2)-(3.3) and Theorem 5.2 in Section 5.2 of Chapter 5, we finally obtain

$$\lim_{n\to\infty} \det(A_n - \lambda I_n) = y_1(T,\lambda) + y_2'(T,\lambda) - 2 = \det(A - \lambda I).$$

Example 3.1. Corollary 2.2 and Theorem 3.2 can be used to compute $\operatorname{Tr} e^{-\frac{1}{\hbar}TH}$ for the harmonic oscillator $H = \frac{1}{2m}(P^2 + m^2\omega^2 Q^2)$. We have

$$\operatorname{Tr} e^{-\frac{1}{\hbar}TH} = \frac{1}{\sqrt{\det A_{i\omega}}}$$

where $A_{i\omega} = -D^2 + \omega^2$, and by formula (5.20) in Section 5.2 of Chapter 5,

$$\operatorname{Tr} e^{-\frac{1}{\hbar}TH} = \frac{1}{2\sinh\frac{\omega T}{2}} \tag{3.4}$$

Of course, since the eigenvalues are $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$, we can get the same result by using geometric series

$$\operatorname{Tr} e^{-\frac{1}{\hbar}TH} = \sum_{n=0}^{\infty} e^{-\frac{1}{\hbar}TE_n} = e^{-\frac{\omega T}{2}} \sum_{n=0}^{\infty} e^{-\omega Tn} = \frac{1}{2\sinh\frac{\omega T}{2}}.$$

Similar results hold for the general second order differential operator $A = -D^2 + v(t)D + u(t)$ on the interval $[0, T]$ with periodic boundary conditions.

Theorem 3.3. Suppose that $\det A > 0$, where $A = -D^2 + v(t)D + u(t)$. Then

$$\int_{\mathcal{L}} e^{-\frac{m}{2\hbar}\int_0^T \left(v(t)\dot{y}(t)y(t) + u(t)y^2(t)\right)dt} d\mu_W^{\text{loop}}(y) = \frac{1}{\sqrt{\det A}}$$

Example 3.2. Let $A = -D^2 + \omega D$. It follows from Theorem 3.3 and (2.6) that for $\varepsilon > 0$

$$\begin{aligned}
\frac{1}{\sqrt{\det(A + \varepsilon I)}} &= \int_{\mathcal{L}} e^{-\frac{m}{2\hbar}\int_0^T \left(\omega\dot{y}(t)y(t) + \varepsilon y^2(t)\right)dt} d\mu_W^{\text{loop}}(y) \\
&= \sqrt{\frac{m}{2\pi\hbar T}} \int_{-\infty}^{\infty} e^{-\frac{mT}{2\hbar}\varepsilon x^2} dx \int_{\mathcal{L}_0} e^{-\frac{m}{2\hbar}\int_0^T \left(\omega\dot{y}_0(t)y_0(t) + \varepsilon y_0^2(t)\right)dt} d\mu_W^{\text{loop}}(y_0) \\
&= \frac{1}{T\sqrt{\varepsilon}} \int_{\mathcal{L}_0} e^{-\frac{m}{2\hbar}\int_0^T \left(\omega\dot{y}_0(t)y_0(t) + \varepsilon y_0^2(t)\right)dt} d\mu_W^{\text{loop}}(y_0)
\end{aligned}$$

where we have used the decomposition $y(t) = x + y_0(t)$, $\int_0^T y_0(t)dt = 0$. Here $\mathcal{L}_0$ is the subset of the free loop space $\mathcal{L}$ which consists of loops with zero constant term in the Fourier series expansion. Using Corollary 5.4 in Section 5.2 of Chapter 5, we obtain

$$\begin{aligned}
\int_{\mathcal{L}_0} e^{-\frac{m}{2\hbar}\int_0^T \omega\dot{y}_0(t)y_0(t)dt} d\mu_W^{\text{loop}}(y_0) &= \lim_{\varepsilon\to 0} \frac{T\sqrt{\varepsilon}}{\sqrt{\det(A + \varepsilon I)}} = \frac{T}{\sqrt{\det' A}} \\
&= \left(\frac{\frac{\omega T}{2}}{\sinh\frac{\omega T}{2}}\right)^{\frac{1}{2}} \qquad (3.5)
\end{aligned}$$

We will use this result in Section 2.2 of Chapter 8.

Problem 3.

1. Derive formula (3.4) using (2.5).

Problem 3.

2. Prove Theorem 3.3.

4.4 Fermionic Systems

(maybe later I'll put it to the section of methods)

4.4.1 1. Canonical Anticommutation Relations

1.1. Motivation.

In Sections 2.6 and 2.7 of Chapter 2 we have shown that the Hilbert space $\mathscr{H} \simeq L^2(\mathbb{R}, dq)$ of a one-dimensional quantum particle can be described in terms of the creation and annihilation operators. Namely, the operators [1]

$$a^* = \frac{1}{\sqrt{2\hbar}}(Q - iP) \quad \text{and} \quad a = \frac{1}{\sqrt{2\hbar}}(Q + iP)$$

satisfy the canonical commutation relation

$$[a, a^*] = I$$

on $W^{2,2}(\mathbb{R}) \cap \hat{W}^{2,2}(\mathbb{R})$, and the vectors

$$\psi_k = \frac{(a^*)^k}{\sqrt{k!}}\psi_0, \quad k = 0, 1, 2, ...$$

where $\psi_0(q) = (\pi\hbar)^{-\frac{1}{4}} e^{-\frac{1}{2\hbar}q^2} \in \mathscr{H}$ satisfies $a\psi_0 = 0$, form an orthonormal basis for $\mathscr{H}$. The corresponding operator $N = a^*a$ is self-adjoint and has an integer spectrum,

$$N\psi_k = k\psi_k, \quad k = 0, 1, 2, ...$$

Similarly, for several degrees of freedom $\mathscr{H} \simeq L^2(\mathbb{R}^n, d^n\boldsymbol{q})$, the creation and annihilation operators are given by

$$a_k^* = \frac{1}{\sqrt{2\hbar}}(Q_k - iP_k) \quad \text{and} \quad a_k = \frac{1}{\sqrt{2\hbar}}(Q_k + iP_k), \quad k = 1, ..., n \tag{1.1}$$

and satisfy canonical commutation relations

$$[a_k, a_l] = [a_k^*, a_l^*] = 0 \quad \text{and} \quad [a_k, a_l^*] = \delta_{kl} I, \quad k, l = 1, ..., n. \tag{1.2}$$

The ground state, the vector $\psi_0(\boldsymbol{q}) = (\pi\hbar)^{-\frac{n}{4}} e^{-\frac{1}{2\hbar}q^2} \in \mathscr{H}$, has the property

$$a_k\psi_0 = 0, \quad k = 1, ..., n$$

and the vectors

$$\psi_{k_1,...,k_n} = \frac{(a_1^*)^{k_1} ... (a_n^*)^{k_n}}{\sqrt{k_1!...k_n!}}\psi_0, \quad k_1, ..., k_n = 0, 1, 2, ...$$

form an orthonormal basis for $\mathscr{H}$. The operator $N = \sum_{k=1}^n a_k^* a_k$ is selfadjoint and has an integer spectrum:

$$N\psi_{k_1,...,k_n} = (k_1 + \cdots + k_n)\,\psi_{k_1,...,k_n}$$

and the Hilbert space $\mathscr{H}$ decomposes into the direct sum of invariant subspaces

$$\mathscr{H} = \bigoplus_{k=0}^{\infty} \mathscr{H}_k \tag{1.3}$$

- the eigenspaces for the operator N.

However spin operators, introduced in Chapter 4, satisfy algebraic relations of different type. Namely, consider the operators $\sigma_\pm = \frac{2}{\hbar}S_\pm = \frac{2}{\hbar}(S_1 \pm iS_2)$, where S_1 and S_2 are spin operators of a quantum particle of spin $\frac{1}{2}$ (see Section 1.1 of Chapter 4). Using the explicit representation of spin operators by Pauli matrices, we get

[01] Here in comparison with Section 2.6 of Chapter 2 we put $\omega = 1$.

$$\sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

The operators $\sigma_\pm$are nilpotent, $\sigma_\pm^2 = 0$, and satisfy the anticommutation relation

$$\sigma_+\sigma_- + \sigma_-\sigma_+ = I_2$$

where I_2 is the identity operator in $\mathbb{C}^2$. Introducing the notion of an anticommutator of two operators,

$$[A, B]_+ = AB + BA$$

we see that the operators $a = \sigma_-$and $a^* = \sigma_+$satisfy canonical anticommutation relations

$$[a, a]_+ = [a^*, a^*]_+ = 0 \quad \text{and} \quad [a, a^*]_+ = I_2.$$

The vector $e_0 = \binom{0}{1}$ has the property $ae_0 = 0$, and together with the vector $a^*e_0 = \binom{1}{0}$ they form an orthonormal basis of $\mathbb{C}^2$. The matrix

$$N = a^*a = \frac{1}{2}(\sigma_3 + I_2) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

has eigenvectors e_0 and a^*e_0 with eigenvalues 0 and 1 . Thus in complete analogy with the previous discussion, we say that a and a^* are fermion creation and annihilation operators for the case of one degree of freedom. The Hilbert space of a Fermi particle is $\mathscr{H} = \mathbb{C}^2$, and the vector e_0 is the ground state.

It is straightforward to generalize this construction to the case of several degrees of freedom. Namely, canonical anticommutation relations have the form

$$[a_k, a_l]_+ = [a_k^*, a_l^*]_+ = 0 \quad \text{and} \quad [a_k, a_l^*]_+ = \delta_{kl} I, \quad k, l = 1, ..., n, \tag{1.4}$$

where I is the identity operator, and creation operators a_j^* are adjoint to annihilation operators a_j in the fermion Hilbert space $\mathscr{H}_F$. Canonical anticommutation relations (1.4) can be realized in the Hilbert space $\mathscr{H}_F = (\mathbb{C}^2)^{\otimes n} = \mathbb{C}^{2^n}$ as follows:

$$a_k = \underbrace{\sigma_3 \otimes \cdots \otimes \sigma_3}_{k-1} \otimes a \otimes I_2 \otimes \cdots \otimes I_2, \tag{1.5}$$

$$a_k^* = \underbrace{\sigma_3 \otimes \cdots \otimes \sigma_3}_{k-1} \otimes a^* \otimes I_2 \otimes \cdots \otimes I_2, \tag{1.6}$$

$k = 1, ..., n$. The ground state, the vector $\psi_0 = e_0 \otimes \cdots \otimes e_0 \in \mathscr{H}_F$, satisfies

$$a_k\psi_0 = 0, \quad k = 1, ..., n, \tag{1.7}$$

and the vectors

$$\psi_{k_1,...,k_n} = (a_1^*)^{k_1} ... (a_n^*)^{k_n} \psi_0, \quad k_1, ..., k_n = 0, 1, \tag{1.8}$$

form an orthonormal basis for $\mathscr{H}_F$. The operator

$$N = \sum_{k=1}^{n} a_k^* a_k$$

is self-adjoint and has an integer spectrum:

$$N\psi_{k_1,...,k_n} = (k_1 + \cdots + k_n)\,\psi_{k_1,...,k_n},$$

and the Hilbert space $\mathscr{H}_F$ decomposes into the direct sum of invariant subspaces

$$\mathscr{H}_F = \bigoplus_{k=0}^{n} \mathscr{H}_k \tag{1.9}$$

- the eigenspaces of N.

Remark. The fermion Hilbert space $\mathscr{H}_F$ is isomorphic to the spin part of the Hilbert space of n quantum particles of spin $\frac{1}{2}$, discussed in Section 3.1 of Chapter 4. The corresponding fermion creation and annihilation operators can also be used for describing spin degrees of freedom. The fundamental importance of the fermion and boson Hilbert spaces - $\mathscr{H}_F = (\mathbb{C}^2)^{\otimes n}$ and
$\mathscr{H}_B = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ - manifests itself in quantum field theory, which formally corresponds to the case $n = \infty$, and describes quantum systems with infinitely many degrees of freedom.

Lemma 1.1. Realization (1.5)-(1.6) of canonical anticommutation relations in the fermion Hilbert space $\mathscr{H}_F$ is irreducible: every operator in $\mathscr{H}_F$, which commutes with all creation and annihilation operators a_k^* and a_k, is a multiple of the identity operator.

Proof. It is sufficient to show that if $\{0\} \neq V \subseteq \mathscr{H}_F$ is an invariant subspace for all operators a_k and a_k^*, then $V = \mathscr{H}_F$. Indeed, every non-zero $\psi \in V$ can be written in the form

$$\psi = \sum_{k_1,...,k_n=0,1} c_{k_1,...,k_n}\psi_{k_1,...,k_n}$$

and let $c_{k_1,...,k_n}\psi_{k_1,...,k_n}$ be any of its non-zero components with maximal degree $k_1+\cdots+k_n$. Using canonical anticommutation relations and (1.7), we obtain

$$a_n^{k_n}...a_1^{k_1}\psi = c\psi_0, \quad c = c_{k_1,...,k_n} \neq 0$$

so that $\psi_0 \in V$. Applying creation operators to ψ_0, we get $V = \mathscr{H}_F$.
Remark. The realization of canonical anticommutation relations in the fermion Hilbert space $\mathscr{H}_F$ is analogous to the representation by the occupation numbers of canonical commutation relations, discussed in Section 2.7 of Chapter 2, and is called representation by the occupation numbers for fermions. It should be emphasized that the algebraic structure of the former relations allows their realization in a finite-dimensional Hilbert space, while the algebraic structure of the latter relations warrants the infinitedimensional Hilbert space.

Analogously to (1.1), coordinate and momentum operators for fermions are defined by

$$Q_k = \sqrt{\frac{\hbar}{2}}\,(a_k + a_k^*), \quad P_k = -i\sqrt{\frac{\hbar}{2}}\,(a_k - a_k^*), \quad k = 1, ..., n. \tag{1.10}$$

As follows from (1.4), they satisfy the following anticommutation relations:

$$[Q_k, Q_l]_+ = [P_k, P_l]_+ = \hbar\delta_{kl}I \quad \text{and} \quad [P_k, Q_l]_+ = 0, \quad k, l = 1, ..., n \tag{1.11}$$

- a fermion analog of Heisenberg commutations relations, introduced in Section 2.1 of Chapter 2. The following result is a fermion analog of the Stone-von Neumann theorem from Section 3.1 of Chapter 2.

Theorem 1.1. Every irreducible finite-dimensional representation of canonical anticommutation relations is unitarily equivalent to the representation by occupation numbers in the fermion Hilbert space $\mathscr{H}_F$.

Proof. Let V be the Hilbert space which realizes the irreducible representation of canonical anticommutation relations (1.4). First of all, there is $\varphi_0 \in V, \|\varphi_0\| = 1$, such that

$$a_1\varphi_0 = \cdots = a_n\varphi_0 = 0$$

Indeed, choose any non-zero $\varphi \in V$; if $a_1\varphi \neq 0$, replace it by the vector $a_1\varphi$, which obviously satisfies $a_1(a_1\varphi_1) = 0$. If $a_2(a_1\varphi) \neq 0$, replace it by $a_2a_1\varphi$, which is annihilated by a_1 and a_2, etc. In finitely many steps we arrive at a non-zero vector $\tilde{\varphi}$ annihilated by the operators $a_1, ..., a_n$, and $\varphi_0 = \tilde{\varphi}/\|\tilde{\varphi}\|$. Now consider the subspace V_0 of V, spanned by the vectors

$$\varphi_{k_1,...,k_n} = (a_1^*)^{k_1} ... (a_n^*)^{k_n} \varphi_0, \quad k_1, ..., k_n = 0, 1$$

It follows from (1.4) that V_0 is an invariant subspace for all operators a_k and a_k^*, so that $V_0 = V$. Since operators a_k^* and a_k are adjoint with respect to the inner product in V, it is easy to see, again using canonical anticommutation relations (1.4), that vectors $\varphi_{k_1,...,k_n}$ form an orthonormal basis for V. The mapping $V \ni \varphi_{k_1,...,k_n} \mapsto \psi_{k_1,...,k_n} \in \mathscr{H}_F$ establishes the Hilbert space isomorphism $V \simeq \mathscr{H}_F$.

Problem 1.1. Express the spin operators $S_j^{(k)}$ of the k-th particle in the system of n spin $\frac{1}{2}$ particles (see Section 3.1 of Chapter 4) in terms of fermion creation and annihilation operators in $\mathscr{H}_F$.

1.2. Clifford algebras. We have seen in Section 2.1 of Chapter 2 that the Heisenberg Lie algebra is the fundamental mathematical structure associated with canonical commutation relations. Similarly, the fundamental mathematical structure associated with the canonical anticommutation relations is Clifford algebra.

Let V be a finite-dimensional vector space over the field k of characteristic zero, and let $Q : V \to k$ be a symmetric non-degenerate quadratic form on V, i.e., $Q(v) = \Phi(v, v), v \in V$, where $\Phi : V \otimes_k V \to k$ is a symmetric non-degenerate bilinear form. The pair (V, Q) is called quadratic vector space.

Definition. A Clifford algebra $C(V, Q) = C(V)$ associated with a quadratic vector space (V, Q) is a k-algebra generated by the vector space V with relations

$$v^2 = Q(v) \cdot 1, \quad v \in V$$

Equivalently, Clifford algebra is defined as a quotient algebra

$$C(V) = T(V)/J$$

where J is a two-sided ideal in the tensor algebra $T(V)$ of V, generated by the elements $u \otimes v + v \otimes u - 2\Phi(u, v) \cdot 1$ for all $u, v \in V$, and 1 is the unit
in $T(V)$. In terms of a basis $\{e_i\}_{i=1}^n$ of V, the Clifford algebra $C(V)$ is a k-algebra with the generators $e_1, ..., e_n$, satisfying the relations

$$[e_i, e_j]_+ = e_ie_j + e_je_i = 2\Phi(e_i, e_j) \cdot 1, \quad i, j = 1, ..., n$$

When $k = \mathbb{C}$ (or any algebraically closed field of characteristic zero), there always exists an orthonormal basis for V - a basis $\{e_i\}_{i=1}^n$ such that $\Phi(e_i, e_k) = \delta_{ik}$. In this case for every dimension n there is one (up to an isomorphism) Clifford algebra C_n with generators $e_1, ..., e_n$ and relations

$$e_i e_j + e_j e_i = 2\delta_{ij} \cdot 1, \quad i, k = 1, ..., n.$$

Remark. If $k = \mathbb{R}$, there exist non-negative integers $p + q = n$ and an isomorphism $V \simeq \mathbb{R}^n$ such that

$$Q(\boldsymbol{x}) = x_1^2 + \cdots + x_p^2 - x_{p+1}^2 - \cdots - x_n^2, \quad \boldsymbol{x} \in \mathbb{R}^n$$

This classifies Clifford algebras over $\mathbb{R}$.

Definition. A left module S for a Clifford algebra $C(V)$ is a finite-dimensional k-vector space S with the linear map $\rho : C(V) \otimes S \to S$ such that

$$\rho(ab \otimes s) = \rho(a \otimes \rho(b \otimes s))$$

for all $a, b \in C(V)$ and $s \in S$.

The fermion Hilbert space $\mathscr{H}_F$, introduced in the previous section, is an irreducible C_{2n}-module. Indeed, it follows from canonical anticommutation relations (1.4) that self-adjoint operators

$$\gamma_{2k-1} = a_k + a_k^*, \tag{1.12}$$

$$\gamma_{2k} = -i\,(a_k - a_k^*)\,, \quad k = 1, ..., n, \tag{1.13}$$

satisfy the relations

$$\gamma_\mu \gamma_\nu + \gamma_\nu \gamma_\mu = 2\delta_{\mu\nu} I, \quad \mu, \nu = 1, ..., 2n \tag{1.14}$$

where I is the identity operator in $\mathscr{H}_F$. We define the action of the Clifford algebra C_{2n} on $\mathscr{H}_F$ by setting

$$\rho(1) = I \quad \text{and} \quad \rho\,(e_\mu) = \gamma_\mu, \quad \mu = 1, ..., 2n,$$

and extending it to a $\mathbb{C}$-algebra homomorphism $\rho : C_{2n} \to \mathrm{End}\,(\mathscr{H}_F)$. Relations (1.14) show that the map ρ admits such an extension.

Proposition 1.1. The homomorphism $\rho : C_{2n} \to \mathrm{End}\,(\mathscr{H}_F)$ is a $\mathbb{C}$-algebra isomorphism.

Proof. It follows from Lemma 1.1 that the representation ρ is irreducible: every operator in $\mathscr{H}_F$ which commutes with all elements of the $\mathbb{C}$-algebra $\rho\,(C_{2n})$ is a multiple of the identity operator. Then by Wedderburn's theorem $\rho\,(C_{2n}) = \mathrm{End}\,(\mathscr{H}_F)$, and since $\dim C_{2n} = 2^{2n} = \dim \mathrm{End}\,(\mathscr{H}_F)$, the map ρ is an isomorphism.

Remark. The structure of a Clifford algebra with an odd number of generators is different. Thus the mapping $\rho\,(e_k) = \sigma_k$, where $\sigma_k, k = 1, 2, 3$, are Pauli matrices (see Section 1 of Chapter 4), defines an irreducible representation of C_3 in $\mathscr{H}_F = \mathbb{C}^2$. However, in this case $C_3 \simeq \mathrm{End}\,(\mathbb{C}^2) \otimes \mathbb{C}[\varepsilon]$, where $\varepsilon = ie_1e_2e_3$ and satisfies $\varepsilon^2 = 1$.

We define the chirality operator by $\Gamma = e^{\pi i N}$, where $N = \sum_{j=1}^n a_j^* a_j$. Since the operator N has an integral spectrum, $\Gamma^2 = I$. Moreover, we have

$$[\Gamma, \gamma_\mu]_+ = 0, \quad \mu = 1, ..., 2n. \tag{1.15}$$

Indeed, as follows from (1.4),

$$N a_j^* = a_j^*(N + I) \quad \text{and} \quad N a_j = a_j(N - I),$$

so that

$$e^{\pi i N} a_j^* = a_j^* e^{\pi i (N+I)} = -a_j^* e^{\pi i N} \quad \text{and} \quad e^{\pi i N} a_j = a_j e^{\pi i (N-I)} = -a_j e^{\pi i N}$$

Thus Γ anticommutes with all a_j, a_j^*, and hence with all γ_μ. Since $\Gamma^2 = I$, the operators

$$P_\pm = \frac{1}{2}(I \pm \Gamma)$$

are orthogonal projection operators and we have a decomposition

$$\mathscr{H}_F = \mathscr{H}_F^+ \oplus \mathscr{H}_F^{--}$$

into the subspaces of positive and negative chirality spinors. It follows from (1.15) that

$$\gamma_\mu \left(\mathscr{H}_F^+\right) = \mathscr{H}_F^-, \quad \mu = 1, ..., 2n.$$

Also, since $e^{\pi i a_j^* a_j} = I - 2a_j^* a_j = -i\gamma_{2j-1}\gamma_{2j}$, we have

$$\Gamma = (-i)^n \gamma_1 ... \gamma_{2n}.$$

Remark. When $n = 2, 4 \times 4$ matrices $\gamma_1, \gamma_2, \gamma_3, \gamma_4$ are celebrated Dirac gamma matrices (for the Euclidean metric on $\mathbb{R}^4$), and $\Gamma = \gamma_5$.

Problem 1.2. Show that the definition of a Clifford algebra $C(V)$ is compatible with the field change: if $k \subset K$ is a field extension and $V_K = K \otimes_k V_k$, then

$$C(V_K) = K \otimes_k C(V_k).$$

Problem 1.3. Let $\mathbb{C} \cdot 1 = C^0 \subset C^1 \subset \cdots \subset C^n = C(V)$ be the natural filtration of a Clifford algebra $C(V)$, where C^r is spanned by the elements $v_1 ... v_s, s \leq r$. Let

$$C^{\mathrm{gr}}(V) = \bigoplus_{k=1}^{n} C^k / C^{k-1}$$

be the associated graded algebra. Show that the skew-symmetrizer map

$$v_1 \wedge \cdots \wedge v_r \mapsto \frac{1}{r!} \sum_{\sigma \in \mathrm{Sym}_r} (-1)^{\varepsilon(\sigma)} v_{\sigma(1)} ... v_{\sigma(r)}$$

establishes a $\mathbb{Z}$-graded algebra isomorphism $\Lambda^\bullet(V) \simeq C^{gr}(V)$, where $\Lambda^\bullet(V)$ is the exterior algebra of V.

Problem 1.4. Formulate and prove the analog of Proposition 1.1 for Clifford algebras with an odd number of generators.

4.4.2 2. Grassmann Algebras

Grassmann algebras - algebras with anticommuting generators - are necessary for the semi-classical description of fermions. The corresponding mathematical definition is the following.

Definition. A Grassmann algebra with n generators is a $\mathbb{C}$-algebra Gr_n with the generators $\theta_1, ..., \theta_n$ satisfying the relations

$$\theta_i \theta_j + \theta_j \theta_i = 0, \quad i, j = 1, ..., n$$

In particular, these relations imply that generators of a Grassmann algebra are nilpotent: $\theta_1^2 = \cdots = \theta_n^2 = 0$. Equivalently,

$$\mathrm{Gr}_n = \mathbb{C}\langle \theta_1, ..., \theta_n \rangle / J$$

- a quotient of a free $\mathbb{C}$-algebra $\mathbb{C}\langle\theta_1, ..., \theta_n\rangle$, generated by $\theta_1, ..., \theta_n$, by the two-sided ideal J generated by the elements $\theta_i\theta_j + \theta_j\theta_i, i, j = 1, ..., n$.
  Remark. It follows from (1.11) that in the semi-classical limit $\hbar \to 0$ fermion operators P_k and $Q_k, k = 1, ..., 2n$, satisfy the defining relations of Grassmann algebra Gr_{2n}.

Comparison with the polynomial algebra

$$\mathbb{C}[x_1, ..., x_n] = \mathbb{C}\langle x_1, ..., x_n\rangle / I$$

- a quotient of a free $\mathbb{C}$-algebra $\mathbb{C}\langle x_1, ..., x_n\rangle$ by the two-sided ideal generated by the elements $x_ix_j - x_jx_i, i, j = 1, ..., n$ - shows that the Grassmann algebra Gr_n can also be considered as a polynomial algebra in anticommuting variables $\theta_1, ..., \theta_n$. In what follows we will always use Roman letters for commuting variables and Greek letters for anticommuting variables, so that

$$\mathrm{Gr}_n = \mathbb{C}[\theta_1, ..., \theta_n].$$

Needless to say, the polynomial algebra $\mathbb{C}[x_1, ..., x_n]$ is isomorphic to the symmetric algebra of the vector space spanned by $x_1, ..., x_n$, and the Grassmann algebra $\mathbb{C}[\theta_1, ..., \theta_n]$ is isomorphic to the exterior algebra $\Lambda^\bullet V$ of the vector space $V = \mathbb{C}\theta_1 \oplus \cdots \oplus \mathbb{C}\theta_n$ with the basis $\theta_1, ..., \theta_n$.

The Grassmann algebra Gr_n is a complex vector space of dimension 2^n and is $\mathbb{Z}$-graded: it admits a decomposition

$$\mathrm{Gr}_n = \bigoplus_{k=0}^{n} \mathrm{Gr}_n^k \tag{2.1}$$

into homogeneous components Gr_n^k of degree k and dimension $\binom{n}{k}, k = 0, ..., n$, where $\mathrm{Gr}_n^0 = \mathbb{C} \cdot 1$. Namely, denote by $|\cdot|$ the degree of homogeneous elements in the Grassmann algebra, $|\alpha| = k$ for $\alpha \in \mathrm{Gr}_n^k$. Then multiplication in Gr_n satisfies $\mathrm{Gr}_n^k \cdot \mathrm{Gr}_n^l \subset \mathrm{Gr}_n^{k+l}$, where $\mathrm{Gr}_n^{k+l} = 0$ if $k + l > n$, and is graded-commutative:

$$\alpha\beta = (-1)^{|\alpha||\beta|}\beta\alpha \tag{2.2}$$

for homogenous elements $\alpha, \beta \in \mathrm{Gr}_n$. The elements of the Grassmann algebra Gr_n of even degree are called even elements, and those of odd degree odd elements.

2.1. Realization of canonical anticommutation relations.

The Grassmann algebra provides us with the explicit representation of canonical anticommutation relations by multiplication and differentiation operators, which is analogous to the holomorphic representation for canonical commutation relations (see Section 2.7 of Chapter 2). Namely, let

$$\partial_i = \frac{\partial}{\partial\theta_i} : \mathrm{Gr}_n \to \mathrm{Gr}_n$$

be left partial differentiation operators, defined on homogeneous monomials $\theta_{i_1}...\theta_{i_k}$ by

$$\frac{\partial}{\partial\theta_i}\theta_{i_1}...\theta_{i_k} = \sum_{l=1}^{k}(-1)^{l-1}\delta_{ii_l}\theta_{i_1}...\check{\theta}_{i_l}...\theta_{i_k}$$

where $\check{\theta}_{i_l}$ denotes the omission of the factor θ_{i_l}. The differentiation operators are of degree -1 and satisfy the graded Leibniz rule,

$$\frac{\partial}{\partial\theta_i}(\alpha\beta) = \frac{\partial\alpha}{\partial\theta_i}\beta + (-1)^{|\alpha|}\alpha\frac{\partial\beta}{\partial\theta_i}.$$

Remark. One can also introduce right partial differentiation operators by

$$(\theta_{i_1}...\theta_{i_k})\,\frac{\partial}{\partial\theta_i} = \sum_{l=1}^{k}(-1)^{k-l}\delta_{ii_l}\theta_{i_1}...\check{\theta}_{i_l}...\theta_{i_k},$$

which satisfy the following graded Leibniz rule:

$$(\alpha\beta)\frac{\partial}{\partial\theta_i} = \alpha\left(\beta\frac{\partial}{\partial\theta_i}\right) + (-1)^{|\beta|}\left(\alpha\frac{\partial}{\partial\theta_i}\right)\beta.$$

To distinguish between the left and right partial derivatives of $f \in \mathrm{Gr}_n$, we will denote them, respectively, by $\frac{\partial}{\partial\theta_i}f$ and $f\frac{\partial}{\partial\theta_i}$.

As a complex vector space, Grassmann algebra Gr_n carries a standard inner product defined by the property that homogeneous monomials $\theta_{i_1}...\theta_{i_k}$, for all $1 \le i_1 < \cdots < i_k \le n$, form an orthonormal basis,

$$(\theta_{i_1}...\theta_{i_k}, \theta_{j_1}...\theta_{j_l}) = \delta_{kl}\delta_{i_1j_1}...\delta_{i_kj_k}. \tag{2.3}$$

By checking on homogeneous monomials, it is elementary to verify that

$$(\partial_i f, g) = \left(f, \hat{\theta}_i g\right), \quad f, g \in \mathrm{Gr}_n$$

where $\hat{\theta}_i$ are left-multiplication by θ_i operators in Gr_n, so that $\hat{\theta}_i = \partial_i^*$. It is also easy to verify that the operators $\hat{\theta}_i$ and ∂_i satisfy the anticommutation relations

$$\left[\hat{\theta}_i, \hat{\theta}_j\right]_+ = [\partial_i, \partial_j]_+ = 0 \quad \text{and} \quad \left[\hat{\theta}_i, \partial_j\right]_+ = \delta_{ij}I, \quad i, j = 1, ..., n$$

where I is an identity operator in Gr_n. Thus we have the following result.

Proposition 2.1. The assignment

$$\mathscr{H}_F \ni \psi_{k_1,...,k_n} \mapsto \theta_1^{k_1}...\theta_n^{k_n} \in \mathrm{Gr}_n$$

establishes an isomorphism $\mathscr{H}_F \simeq \mathrm{Gr}_n$ between the fermion Hilbert space of n identical particles, and the vector space of the Grassmann algebra with n generators. It preserves decompositions (1.9) and (2.1) and has the property that

$$a_i^* \mapsto \hat{\theta}_i \quad \text{and} \quad a_i \mapsto \frac{\partial}{\partial\theta_i}, \quad i = 1, ..., n.$$

Using Proposition 2.1, it is also very easy to verify that the representation of canonical anticommutation relations in the fermion Hilbert space $\mathscr{H}_F$ is irreducible. Indeed, suppose that $B \in \mathrm{End}\,(\mathrm{Gr}_n)$ commutes with all operators $\hat{\theta}_i$ and ∂_i. Then

$$\partial_i(B(1)) = B\,(\partial_i(1)) = 0, \quad i = 1, ..., n.$$

The only solution of the equations $\partial_1 f = \cdots = \partial_n f = 0$ is $f = c \cdot 1$, so that $B(1) = c \cdot 1$. Since B commutes with all creation operators $\hat{\theta}_i$, we obtain $B = cI$.

Remark. We will show in Section 2.3 that by using the notion of Berezin integral, the inner product (2.3) in Gr_n can be written in a form (2.11), which is similar to the definition of the inner product in the holomorphic representation, given by formula (2.52) in Section 2.7 of

Chapter 2.
2.2. Differential forms. An algebra of differential forms in anticommuting variables $\theta_1, ..., \theta_n$ is a $\mathbb{C}$-algebra $\Omega_n^\bullet$ with odd generators $\theta_1, ..., \theta_n$ and even generators $d\theta_1, ..., d\theta_n$ satisfying relations

$$\theta_i \cdot d\theta_j = d\theta_j \cdot \theta_i, \quad i, j = 1, ..., n$$

Equivalently, $\Omega_n^\bullet$ is a symmetric tensor product over $\mathbb{C}$ of Grassmann algebra Gr_n and polynomial algebra $\mathbb{C}[d\theta_1, ..., d\theta_n]$, and every $\omega \in \Omega_n^\bullet$ can be uniquely written as

$$\omega = \sum_{k=0}^{\infty} f_k (d\theta_1)^{k_1} \cdots (d\theta_n)^{k_n}, \quad f_k \in \mathrm{Gr}_n \tag{2.4}$$

where $\boldsymbol{k} = (k_1, ..., k_n)$ is a multi-index and $f_{\boldsymbol{k}} = 0$ for all $\boldsymbol{k}$, except finitely many. By definition, the degree $|\omega_{\boldsymbol{k}}|$ of a homogeneous component $\omega_{\boldsymbol{k}} = f_k (d\theta_1)^{k_1} \cdots (d\theta_n)^{k_n} \in \Omega_n^\bullet$ is $|f_k|$, the degree of $f_k \in \mathrm{Gr}_n$.

Remark. It is instructive to compare the algebra $\Omega_n^\bullet$ with the algebra of polynomial differential forms on $\mathbb{C}^n$. On the one hand, $\Omega_n^\bullet$ is an infinitedimensional algebra in commuting variables $d\theta_1, ..., d\theta_n$ with coefficients in a finite-dimensional algebra Grassmann algebra $\mathbb{C}[\theta_1, ..., \theta_n]$. On the other hand, the algebra of differential forms in commuting variables $x_1, ..., x_n$ is a finite-dimensional algebra in anticommuting variables $dx_1, ..., dx_n$ with coefficients in an infinite-dimensional polynomial algebra $\mathbb{C}[x_1, ..., x_n]$.

The analog of the exterior (de Rham) differential on the algebra $\Omega_n^\bullet$ is the mapping $d : \Omega_n^\bullet \to \Omega_n^\bullet$, defined by

$$d\omega = \sum_{k=0}^{\infty} \sum_{i=1}^{n} \frac{\partial f_k}{\partial \theta_i} d\theta_i (d\theta_1)^{k_1} \cdots (d\theta_n)^{k_n}, \quad f_k \in \mathrm{Gr}_n$$

where ω is given by (2.4). It can also be written as $d = \sum_{i=1}^n d\theta_i \partial_i$, where it is understood that $\partial_i (d\theta_j) = 0$ for all $i, j = 1, ..., n$.

Lemma 2.1. The exterior differential d on $\Omega_n^\bullet$ satisfies the graded Leibniz rule,

$$d(\omega_1 \omega_2) = d\omega_1 \omega_2 + (-1)^{|\omega_1|} \omega_1 d\omega_2$$

for homogeneous ω_1, and is nilpotent, $d^2 = 0$.
Proof. The graded Leibniz rule for d follows from the corresponding property of partial differentiation operators ∂_i. The property $d^2 = 0$ follows from the commutativity of "differentials" $d\theta_i$ and anticommutativity of the partial derivatives ∂_i.

The next result is an analog of the Poincar lemma for differential forms in anticommuting variables.

Lemma 2.2. Suppose that $\omega \in \Omega_n^\bullet$ is closed, $d\omega = 0$. Then ω is exact: there is $\eta \in \Omega_n^\bullet$ such that $\omega = d\eta$.

Definition. A 2 -form $\omega \in \Omega_n^\bullet$,

$$\omega = \frac{1}{2} \sum_{i,j=1}^{n} \omega^{ij} d\theta_i d\theta_j, \quad \omega^{ij} = \omega^{ji} \in \mathrm{Gr}_n \tag{2.5}$$

is called a symplectic form on a Grassmann algebra if it is closed, $d\omega = 0$, and is nondegenerate: the $n \times n$ symmetric matrix $\{\omega^{ij}\}_{i,j=1}^n$ is invertible in Gr_n.

In particular, the 2 -form ω with constant coefficients $\omega^{ij} \in \mathbb{C}$ is always closed, and ω is symplectic if and only if the matrix $\{\omega^{ij}\}_{i,j=1}^n$ is nondegenerate. Since every quadratic form over $\mathbb{C}$ can be written as a sum of squares, we can always assume that generators $\theta_1, ..., \theta_n$ are chosen such that the symplectic form ω with constant coefficients has a canonical form

$$\omega = \frac{1}{2}\sum_{i=1}^{n} d\theta_i d\theta_i. \tag{2.6}$$

With every symplectic form (2.5) there is an associated Poisson bracket on Grassmann algebra, defined by

$$\{f,g\} = \sum_{i,j=1}^{n} \left(f\frac{\partial}{\partial\theta_i}\right)\omega_{ij}\left(\frac{\partial}{\partial\theta_j}g\right), \quad f,g \in \mathrm{Gr}_n \tag{2.7}$$

where $\{\omega_{ij}\}_{i,j=1}^{n}$ is the inverse matrix to $\{\omega^{ij}\}_{i,j=1}^{n}$, and we are using notation for the left and right partial differentiation operators, introduced in the previous section. The following result - an analog of Theorem 2.9 in Section 2.4 of Chapter 1 - is fundamental for formulating Hamiltonian mechanics for the systems with anticommuting variables, which we will discuss in Chapter 8.

Proposition 2.2. Suppose that all coefficients ω^{ij} of a closed symplectic form ω are even. Then the Poisson bracket map

$$\{,\} : \mathrm{Gr}_n \times \mathrm{Gr}_n \to \mathrm{Gr}_n$$

satisfies the following properties.

(i) (Graded skew-symmetry)

$$\{f,g\} = -(-1)^{|f||g|}\{g,f\}.$$

(ii) (Graded Leibniz rule)

$$\{fg,h\} = f\{g,h\} + (-1)^{|f||g|}g\{f,h\}.$$

(iii) (Graded Jacobi identity)

$$\{f,\{g,h\}\} + (-1)^{|f|(|g|+|h|)}\{g,\{h,f\}\} + (-1)^{|h|(|f|+|g|)}\{h,\{f,g\}\} = 0$$

for all $f,g,h \in \mathrm{Gr}_n$.

Proof. Part (i) follows from (2.2), the property

$$\frac{\partial}{\partial\theta_i}f = -(-)^{|f|}f\frac{\partial}{\partial\theta_i}$$

and the condition that coefficients ω^{ij} are even. The graded Leibniz rule follows from the corresponding property of right partial differentiation operators. The graded Jacobi identity for the Poisson bracket

$$\{f,g\} = \sum_{i=1}^{n}\left(f\frac{\partial}{\partial\theta_i}\right)\left(\frac{\partial}{\partial\theta_i}g\right)$$

which corresponds to the canonical symplectic form (2.6), can be verified by a direct computation. The proof of a general case is left to the reader.

Problem 2.1. Complete the proof of Lemma 2.1.

Problem 2.2. Prove Lemma 2.2.

Problem 2.3. Complete the proof of Proposition 2.2.

2.3. Berezin integral. There is a principal difference between differential forms in commuting and in anticommuting variables. The former can be differentiated and integrated, and the differential and integral are related by the Stokes' formula. However, the latter can only be differentiated. Still, there is an analog of the integration over anticommuting variables.

Definition. The integral on a Grassmann algebra Gr_n with an ordered set of generators $\theta_1, ..., \theta_n$ (Berezin integral) is a linear functional $B : \mathrm{Gr}_n \to \mathbb{C}$, defined by

$$B(f) = f^{12...n}$$

where

$$f = \sum_{k=0}^{n} \sum_{1 \le i_1 < \cdots < i_k \le n} f^{i_1 ... i_k} \theta_{i_1} ... \theta_{i_k} \in \mathrm{Gr}_n$$

It is traditional to write the Berezin integral in the form

$$B(f) = \int f(\boldsymbol{\theta}) d\theta_1 ... d\theta_n$$

where $\boldsymbol{\theta} = (\theta_1, ..., \theta_n)$, as if $f = f(\theta_1, ..., \theta_n)$ was actually a "function of anticommuting variables". It follows from the definition of partial differentiation operators that

$$\int f(\boldsymbol{\theta}) d\theta_1 ... d\theta_n = \frac{\partial}{\partial \theta_n} ... \frac{\partial}{\partial \theta_1} f$$

which implies

$$\int \frac{\partial}{\partial \theta_i} f(\boldsymbol{\theta}) d\theta_1 ... d\theta_n = 0.$$

This leads to the following integration by parts formula for the Berezin integral:

$$\int f(\boldsymbol{\theta}) \left(\frac{\partial}{\partial \theta_i} g \right) (\boldsymbol{\theta}) d\theta_1 ... d\theta_n = \int \left(f \frac{\partial}{\partial \theta_i} \right) (\boldsymbol{\theta}) g(\boldsymbol{\theta}) d\theta_1 ... d\theta_n$$

for homogeneous $f, g \in \mathrm{Gr}_n$.

Remark. The Berezin integral is not an integral in the sense of integration theory. It is defined as a linear functional on a Grassmann algebra Gr_n and it depends on the ordering of the generators $\theta_1, ..., \theta_n$ of Gr_n, which is symbolized by $d\theta_1 ... d\theta_n$. For each $\sigma \in \mathrm{Sym}_n$,

$$\int f(\boldsymbol{\theta}) d\theta_1 ... d\theta_n = (-1)^{\varepsilon(\sigma)} \int f(\boldsymbol{\theta}) d\theta_{\sigma(1)} ... d\theta_{\sigma(n)}$$

where $\varepsilon(\sigma)$ is the parity of a permutation σ.

Remark. Using the embeddings $\mathrm{Gr}_k \subset \mathrm{Gr}_n$ for $k \le n$, physicists usually define the Berezin integral as a "repeated integral" starting from the following "one-dimensional integrals":

$$\int d\theta_i = 0, \quad \int \theta_i d\theta_i = 1, \quad i = 1, ..., n$$

Lemma 2.3 (Change of variables for Berezin integral). Let $\theta_1, ..., \theta_n$ and $\tilde{\theta}_1, ..., \tilde{\theta}_n$ be two sets of generators of the Grassmann algebra Gr_n, related by $\theta_i = \sum_{j=1}^{n} a_{ij} \tilde{\theta}_j$, where the $n \times n$ matrix $A = \{a_{ij}\}_{i,j=1}^{n}$ is non-degenerate. Then

$$\int f(\boldsymbol{\theta}) d\theta_1 ... d\theta_n = \frac{1}{\det A} \int \tilde{f}(\tilde{\boldsymbol{\theta}}) d\tilde{\theta}_1 ... d\tilde{\theta}_n$$

where $\tilde{f}(\tilde{\boldsymbol{\theta}}) = f(\boldsymbol{\theta}) = f\left(\sum_{j=1}^{n} a_{1j} \tilde{\theta}_j, ..., \sum_{j=1}^{n} a_{nj} \tilde{\theta}_j \right)$.

Proof. By multi-linear algebra, $\tilde{f}^{12...n} = f^{12...n} \det A$.

Remark. According to the lemma, the "density" $d\theta_1 ... d\theta_n$ has the transformation law

$$d\theta_1 ... d\theta_n = \frac{1}{\det A} d\tilde{\theta}_1 ... d\tilde{\theta}_n \tag{2.8}$$

under the change of variables $\theta_i = \sum_{j=1}^n a_{ij}\tilde{\theta}_j$. This differs from the usual change of variables formula for the Lebesgue integral

$$\int_{\mathbb{R}^n} f(x_1, ..., x_n)\, dx_1 ... dx_n = |\det A| \int_{\mathbb{R}^n} \tilde{f}(y_1, ..., y_n)\, dy_1 ... dy_n \tag{2.9}$$

or $dx_1 ... dx_n = |\det A| dy_1 ... dy_n$, where $x_i = \sum_{j=1}^n a_{ij} y_j$. Of course, the Berezin integral is rather a multiple derivative than an integral with respect to a measure, which explains this profound difference.

Let $A = \{a_{ij}\}_{i,j=1}^n$ be an $n \times n$ skew-symmetric matrix. For even $n = 2m$ its Pfaffian $\mathrm{Pf}(A)$ is defined by

$$\mathrm{Pf}(A) = \frac{1}{m! 2^m} \sum_{\sigma \in \mathrm{Sym}_n} (-1)^{\varepsilon(\sigma)} a_{\sigma(1)\sigma(2)} ... a_{\sigma(n-1)\sigma(n)},$$

where $\varepsilon(\sigma)$ is the parity of a permutation σ. By definition, $\mathrm{Pf}(A) = 0$ when n is odd.

Proposition 2.3 (Gaussian integration for anticommuting variables). Let $A = \{a_{ij}\}_{i,j=1}^n$ be an $n \times n$ skew-symmetric matrix. Then
(i)

$$\int \exp\left\{\frac{1}{2} \sum_{i,j=1}^n a_{ij}\theta_i\theta_j\right\} d\theta_1 ... d\theta_n = \mathrm{Pf}(A)$$

(ii) For any non-degenerate $n \times n$ matrix C

$$\mathrm{Pf}\left(CAC^t\right) = \mathrm{Pf}(A) \det C$$

(iii)

$$\mathrm{Pf}(A)^2 = \det A$$

Proof. Part (i) obviously holds for odd n since the integrand is an even element of Gr_n. By the definition of the Pfaffian, we get for $n = 2m$,

$$\frac{1}{m! 2^m} \left(\sum_{i,j=1}^n a_{ij}\theta_i\theta_j\right)^m = \mathrm{Pf}(A)\theta_1 ... \theta_n$$

and expanding the exponent into power series, we obtain

$$\int \exp\left\{\frac{1}{2} \sum_{i,j=1}^n a_{ij}\theta_i\theta_j\right\} d\theta_1 ... d\theta_n = \mathrm{Pf}(A) \int \theta_1 ... \theta_n d\theta_1 ... d\theta_n = \mathrm{Pf}(A)$$

Part (ii) follows from part (i) and Lemma 2.3. Part (iii) is a classical result, which can be proved by the Berezin integral as follows. Suppose first that A is real-valued. There exists an orthogonal matrix C with determinant 1 such that

$$CAC^{-1} = \begin{pmatrix} 0 & \lambda_1 & \cdots & 0 & 0 \\ -\lambda_1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \lambda_m \\ 0 & 0 & \cdots & -\lambda_m & 0 \end{pmatrix}$$

is a block-diagonal matrix. Using part (ii) with this matrix C, we obtain

$$\mathrm{Pf}(A) = \int e^{\lambda_1\tilde\theta_1\tilde\theta_2+\cdots+\lambda_m\tilde\theta_{2m-1}\tilde\theta_{2m}} d\tilde\theta_1 ... d\tilde\theta_{2m} = \lambda_1 ... \lambda_m$$

so that $\mathrm{Pf}(A)^2 = \det A$. This relation holds for complex-valued A, since both sides are polynomials in variables $a_{ij}, 1 \le i < j \le n$, which coincide for real a_{ij}.

For a Grassmann algebra $\mathrm{Gr}_{2n} = \mathbb{C}\left[\theta_1, ..., \theta_n, \bar\theta_1, ..., \bar\theta_n\right]$ with $2n$ generators denote by $\int d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} = \int d\theta_1 d\bar\theta_1 ... d\theta_n d\bar\theta_n$ the corresponding Berezin integral,

$$\int f(\boldsymbol{\theta}, \overline{\boldsymbol{\theta}}) d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} = \frac{\partial}{\partial\bar\theta_n}\frac{\partial}{\partial\theta_n} ... \frac{\partial}{\partial\bar\theta_1}\frac{\partial}{\partial\theta_1} f, \quad f \in \mathbb{C}\left[\theta_1, ..., \theta_n, \bar\theta_1, ..., \bar\theta_n\right].$$

Lemma 2.4. For any $n \times n$ matrix $A = \{a_{ij}\}_{i,j=1}^n$,

$$\int \exp\left\{\sum_{i,j=1}^n a_{ij}\theta_i\bar\theta_j\right\} d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} = \det A$$

Proof. It follows from the definition of a matrix determinant that

$$\frac{1}{n!}\left(\sum_{i,j=1}^n a_{ij}\theta_i\bar\theta_j\right)^n = \det A \theta_1\bar\theta_1 ... \theta_n\bar\theta_n \tag{2.10}$$

Definition. An involution on a Grassmann algebra Gr_n over $\mathbb{C}$ is a complex anti-linear mapping $\mathrm{Gr}_n \ni f \mapsto f^* \in \mathrm{Gr}_n$ satisfying $(f^*)^* = f$ and $(fg)^* = g^* f^*$ for all $f, g \in \mathrm{Gr}_n$.

The Grassmann algebra $\mathbb{C}\left[\theta_1, ..., \theta_n, \bar\theta_1, ..., \bar\theta_n\right]$ has a natural involution defined on generators by $(\theta_1)^* = \bar\theta_1, \left(\bar\theta_1\right)^* = \theta_1, ..., (\theta_n)^* = \bar\theta_n, \left(\bar\theta_n\right)^* = \theta_n$. In particular, for

$$f(\boldsymbol{\theta}) = \sum_{k=0}^n \sum_{1\le i_1<\cdots<i_k\le n} f^{i_1...i_k}\theta_{i_1}...\theta_{i_k} \in \mathrm{Gr}_n \subset \mathrm{Gr}_{2n}$$

we have

$$f(\boldsymbol{\theta})^* = \overline{f(\boldsymbol{\theta})} = \sum_{k=0}^n \sum_{1\le i_1<\cdots<i_k\le n} \overline{f^{i_1...i_k}}\bar\theta_{i_k}...\bar\theta_{i_1} \in \mathrm{Gr}_{2n}$$

The next lemma expresses the inner product on the Grassmann algebra Gr_n, introduced in Section 2.1, in terms of the Berezin integral.

Lemma 2.5. The standard inner product (2.3) on the Grassmann algebra $\mathrm{Gr}_n = \mathbb{C}[\theta_1, ..., \theta_n]$ is given by the following Berezin integral over the Grassmann algebra $\mathrm{Gr}_{2n} = \mathbb{C}\left[\theta_1, ..., \theta_n, \bar\theta_1, ..., \bar\theta_n\right]$:

$$(f_1, f_2) = \int f_1(\boldsymbol{\theta})\overline{f_2(\boldsymbol{\theta})} e^{-\overline{\boldsymbol{\theta}}\boldsymbol{\theta}} d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} \tag{2.11}$$

where $\overline{\boldsymbol{\theta}}\boldsymbol{\theta} = \bar\theta_1\theta_1 + \cdots + \bar\theta_n\theta_n$.

Proof. Put $f_1(\boldsymbol{\theta}) = \theta_{i_1}...\theta_{i_k}$ and $f_2(\boldsymbol{\theta}) = \theta_{j_1}...\theta_{j_l}$. It is clear that the integral (2.11) is 0, unless $k = l$ and $i_1 = j_1, ..., i_k = j_k$, in which case we have

$$\begin{aligned}(\theta_{i_1}...\theta_{i_k}, \theta_{i_1}...\theta_{i_k}) &= \int \theta_{i_1}...\theta_{i_k}\bar\theta_{i_k}...\bar\theta_{i_1} e^{-\left(\bar\theta_1\theta_1+\cdots+\bar\theta_n\theta_n\right)} d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} \\ &= \int \theta_1...\theta_n\bar\theta_n...\bar\theta_1 d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} \\ &= \int \theta_1\bar\theta_1...\theta_n\bar\theta_n d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} = 1\end{aligned}$$

The following result was already stated in Section 2.1. Lemma 2.5 allows us to prove it in a way that is reminiscent of a holomorphic representation (see Section 2.7 of Chapter 2).

Corollary 2.1. The operators ∂_i and $\hat{\theta}_i, i = 1, ..., n$, are adjoint with respect to the inner product on Gr_n.

Proof. Using Lemma 2.5, formulas $\partial_i \overline{f(\boldsymbol{\theta})} = 0, \partial_i e^{-\overline{\boldsymbol{\theta}}\boldsymbol{\theta}} = \bar{\theta}_i e^{-\overline{\boldsymbol{\theta}}\boldsymbol{\theta}}$, and the integration by parts formula, we obtain

$$\begin{aligned}(\partial_i f_1, f_2) &= \int \partial_i f_1(\boldsymbol{\theta}) \overline{f_2(\boldsymbol{\theta})} e^{-\overline{\boldsymbol{\theta}}\boldsymbol{\theta}} d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} \\ &= -(-1)^{|f_1|+|f_2|} \int f_1(\boldsymbol{\theta}) \overline{f_2(\boldsymbol{\theta})} \bar{\theta}_i e^{-\overline{\boldsymbol{\theta}}\boldsymbol{\theta}} d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} \\ &= -(-1)^{|f_1|+|f_2|} \int f_1(\boldsymbol{\theta}) \overline{\theta_i f_2(\boldsymbol{\theta})} e^{-\overline{\boldsymbol{\theta}}\boldsymbol{\theta}} d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} \\ &= \left(f_1, \hat{\theta}_i f_2\right),\end{aligned}$$

since the last integral and $(f_1, \hat{\theta}_i f_2)$ are both 0 unless $|f_1| + |f_2|$ is odd.

Problem 2.4. Evaluate the Berezin integral

$$\int \exp\left\{\frac{1}{2}\sum_{i,j=1}^{n} a_{ij}\theta_i\theta_j + \sum_{k=1}^{n} \eta_k\theta_k\right\} d\theta_1 ... d\theta_n$$

where $\eta_1, ..., \eta_n$ are Grassmann variables.

Problem 2.5. Prove formula (2.10).

Problem 2.6. Prove that

$$\int f(\boldsymbol{\theta}) e^{-\overline{\boldsymbol{\theta}}\boldsymbol{\theta}} d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} = f(0)$$

- the constant term of expansion of $f(\boldsymbol{\theta})$ into the sum of monomials in $\mathbb{C}[\theta_1, ..., \theta_n]$.

4.4.3 3. Graded Linear Algebra

3.1. Graded vector spaces and superalgebras.

The notions of graded vector spaces and superalgebras, introduced in this section, allow us to consider commuting and anticommuting variables on the same footing.

Definition. A $\mathbb{Z}/2\mathbb{Z}$ graded vector space (graded vector space for brevity, or super vector space) over $\mathbb{C}$ is a vector space W with a decomposition

$$W = W^0 \oplus W^1$$

into even and odd subspaces. The elements in $W^0 \cup W^1 \backslash \{0\}$ are called homogeneous and the parity is a map $|\cdot| : W^0 \cup W^1 \backslash \{0\} \to \{0, 1\}$ such that $|w| = 0$ for $w \in W^0$ and $|w| = 1$ for $w \in W^1$.

We reserve the notation V for ordinary (even) vector spaces, denoting graded vector spaces by W. If W is finite-dimensional, we define graded dimension as a pair $(\dim W^0, \dim W^1)$, usually denoted by $n_0|n_1$, where $n_i = \dim W^i, i = 0, 1$. When $W^0 = \mathbb{C}^p$ and $W^1 = \mathbb{C}^q$, the corresponding graded vector space W is denoted by $\mathbb{C}^{p|q}$. A fermion Hilbert space $\mathscr{H}_F$ is a graded vector space with the even and odd subspaces given by decomposition (1.9):

$$\mathscr{H}_F^0 = \bigoplus_{k \text{ even}} \mathscr{H}_k, \quad \mathscr{H}_F^1 = \bigoplus_{k \text{ odd}} \mathscr{H}_k$$

The graded dimension of $\mathscr{H}_F$ is $2^{n-1}|2^{n-1}$.
Direct sums and tensor products of graded vector spaces are defined in the same way as for ordinary vector spaces. For the direct sums the homogeneous subspaces are defined by

$$(W_1 \oplus W_2)^k = W_1^k \oplus W_2^k, \quad k = 0, 1,$$

and for the tensor products they are defined as

$$(W_1 \otimes W_2)^k = \bigoplus_{i+j=k} W_1^i \otimes W_2^j, \quad k = 0, 1$$

The difference between ordinary and graded vector spaces becomes transparent in the definition of the corresponding tensor categories. Namely, the associativity morphism

$$c_{W_1W_2W_3} : W_1 \otimes (W_2 \otimes W_3) \to (W_1 \otimes W_2) \otimes W_3$$

for graded vector spaces is defined by the same formula

$$c_{W_1W_2W_3}\,(w_1 \otimes (w_2 \otimes w_3)) = (w_1 \otimes w_2) \otimes w_3$$

as in the case of ordinary vector spaces, whereas the commutativity morphism

$$\sigma_{W_1W_2} : W_1 \otimes W_2 \to W_2 \otimes W_1$$

is defined for the homogeneous elements by

$$\sigma_{W_1W_2}\,(w_1 \otimes w_2) = (-1)^{|w_1||w_2|} w_2 \otimes w_1$$

The tensor algebra $T(W)$ of a graded vector space W is defined using the associativity morphism. However the exterior algebra $\Lambda^\bullet W$ and symmetric algebra $\mathrm{Sym}(W)$ of W are defined as quotient algebras of $T(W)$ by using the commutativity morphism. Namely,

$$\mathrm{Sym}(W) = T(W)/I,$$

where I is the two-sided ideal in $T(W)$ generated by $w_1 \otimes w_2 - \sigma\,(w_2 \otimes w_1)$, $w_1, w_2 \in W$, and

$$\Lambda^\bullet(W) = T(W)/J,$$

where J is the two-sided ideal in $T(W)$ generated by $w_1 \otimes w_2 + \sigma\,(w_2 \otimes w_1)$, $w_1, w_2 \in W$. Here $\sigma = \sigma_{W,W}$ is the commutativity morphism.

Definition. Let $W = W^0 \oplus W^1$ be a graded vector space. A parity-reversed vector space ΠW is a graded vector space with $(\Pi W)^0 = W^1$ and $(\Pi W)^1 = W^0$.

It immediately follows from the definitions that for even vector space V

$$\mathrm{Sym}(\Pi V) = \Lambda^\bullet(V) \quad \text{and} \quad \Lambda^\bullet(\Pi V) = \mathrm{Sym}(V) \tag{3.1}$$

Definition. A superalgebra over $\mathbb{C}$ is a graded vector space $A = A^0 \oplus A^1$ with a $\mathbb{C}$-algebra structure such that $1 \in A^0$ and

$$A^0 \cdot A^0 \subset A^0, \quad A^0 \cdot A^1 \subset A^1, \quad A^1 \cdot A^1 \subset A^0$$

A superalgebra A is a commutative superalgebra if

$$a \cdot b = (-1)^{|a||b|} b \cdot a$$

for homogeneous elements $a, b \in A$.
An even superalgebra A is just an ordinary $\mathbb{C}$-algebra.

Definition. A left (super) module for a superalgebra A is a graded vector space M with the linear map

$$A \otimes M \ni a \otimes m \mapsto a \cdot m \in M$$

such that $|a \cdot m| = (|a| + |m|) \bmod 2$ for homogeneous $a \in A$ and $m \in M$, and $ab \cdot m = a \cdot (b \cdot m)$ for all $a, b \in A$ and $m \in M$.

Problem 3.

1. Let $\sigma \in \mathrm{Sym}_n$. Show that the isomorphism

$$W_1 \otimes \cdots \otimes W_n \simeq W_{\sigma^{-1}(1)} \otimes \cdots \otimes W_{\sigma^{-1}(n)},$$

induced by the commutativity morphism of graded vector spaces, is well defined does not depend on the representation of σ as a product of transpositions in Sym_n.

Problem 3.

2. Show that for a graded vector space W the algebras $\mathrm{Sym}(W)$ and $\Lambda^\bullet(W)$ are superalgebras.

3.2. Examples of superalgebras.

Example 3.1 (Tensor algebra). The tensor algebra

$$T(V) = \bigoplus_{k=0}^{\infty} V^{\otimes k}, \quad V^0 = \mathbb{C} \cdot 1,$$

of an even vector space V is a superalgebra. The multiplication is given by the tensor product, and even and odd subspaces - by

$$T(V)^0 = \bigoplus_{k \text{ even}} V^{\otimes k}, \quad T(V)^1 = \bigoplus_{k \text{ odd}} V^{\otimes k}.$$

Example 3.2 (Symmetric algebra). The symmetric algebra $\mathrm{Sym}(V)$ of an even vector space V is a commutative algebra. A choice of a basis $x_1, ..., x_n$ of V establishes the isomorphism $\mathrm{Sym}(V) \simeq \mathbb{C}[x_1, ..., x_n]$ - a polynomial algebra in commuting variables $x_1, ..., x_n$.

Example 3.3 (Exterior algebra). The exterior algebra $\Lambda^\bullet V$ of an even vector space V is a commutative superalgebra, with multiplication given by the wedge product; the even and odd subspaces are images of the corresponding subspaces of $T(V)$ under the surjective mapping

$$T(V) \to \Lambda^\bullet V = T(V)/J$$

where J is the two-sided ideal in $T(V)$, generated by the elements $u \otimes v + v \otimes u$, $u, v \in V$. According to (3.1), $\Lambda^\bullet(V) = \mathrm{Sym}(\Pi V)$. The choice of a basis $\theta_1, ..., \theta_n$ of the odd vector space ΠV establishes the isomorphism

$$\Lambda^\bullet(V) \simeq \mathbb{C}\left[\theta_1, ..., \theta_n\right].$$

Here $\mathbb{C}\left[\theta_1, ..., \theta_n\right]$ is the Grassmann algebra - a polynomial algebra in anticommuting variables $\theta_1, ..., \theta_n$.

Example 3.4 (Algebra of differential forms). Let M be an n-dimensional manifold. The graded algebra $\mathcal{A}^\bullet(M)$ of smooth differential forms on M is a commutative superalgebra.

Example 3.5 (Clifford algebra). The Clifford algebra $C(V)$ of a quadratic vector space (V, Q) is a superalgebra, with the multiplication and grading descending from the tensor algebra $T(V)$ under the surjective mapping

$$T(V) \to \Lambda^\bullet V = T(V)/J,$$

where now J is the two-sided ideal in $T(V)$, generated by the elements $u \otimes v + v \otimes u - 2\Phi(u, v) \cdot 1, u, v \in V$. The natural map $V \hookrightarrow C(V)$ is injective, and V is identified with its image in $C(V)$. The elements of V are odd in $C(V)$. The fermion Hilbert space $\mathscr{H}_F$ is a left supermodule for C_{2n}, and the $\mathbb{C}$-algebra isomorphism $\rho : C_{2n} \to \mathrm{End}\left(\mathscr{H}_F\right)$ (see Proposition 1.1) is an isomorphism of superalgebras.

Example 3.6 (Graded matrix algebra). Let W be a graded vector space. The vector space $\mathrm{End}(W)$ of all endomorphisms of W is a graded vector space: the even subspace consists of all endomorphisms which preserve the grading in W, and the odd subspace consists of those which reverse the grading. The vector space $\mathrm{End}(W)$ is a superalgebra with the product given by the composition of endomorphisms, and W is a module for $\mathrm{End}(W)$. When $W = \mathbb{C}^{p|q}$, the superalgebra $\mathrm{End}(W)$ is usually denoted by $\mathrm{Mat}(p|q)$. Its elements can be conveniently represented by 2×2 block matrices

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

where A_{11}, A_{12}, A_{21}, and A_{22} are, respectively, matrices of orders $p \times p, p \times q$, $q \times p$, and $q \times q$. The even and odd elements of $\mathrm{Mat}(p|q)$ are, respectively, block-diagonal and anti-diagonal matrices $\begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix}$ and $\begin{pmatrix} 0 & A_{12} \\ A_{21} & 0 \end{pmatrix}$.

Example 3.7 (Lie superalgebra). A graded vector space $\mathfrak{g}$ is called a Lie superalgebra (or, super Lie algebra) if it carries a Lie superbracket - a linear mapping $[\,] :, \mathfrak{g} \otimes \mathfrak{g} \to \mathfrak{g}$ satisfying the following properties.

(i) (Super skew-symmetry)

$$[x, y] = -(-1)^{|x||y|}[y, x]$$

for homogeneous $x, y \in \mathfrak{g}$.

(ii) (Super Jacobi identity)

$$[x, [y, z]] + (-1)^{|x|(|y|+|z|)}[y, [z, x]] + (-1)^{|z|(|x|+|y|)}[z, [x, y]] = 0$$

for homogeneous $x, y, z \in \mathfrak{g}$.

According to Proposition 2.2, a Grassmann algebra Gr_n with a Poisson bracket (2.7) is a Lie superalgebra.

Corresponding to classical simple Lie algebras there are associated Lie superalgebras.

Problem 3.

3. Verify all the statements in this section.

Problem 3.

4. Show that a superalgebra A carries a Lie superalgebra structure with a Lie superbracket defined by

$$[a, b] = ab - (-1)^{|a||b|}ba$$

for homogeneous $a, b \in A$.

3.3. Supertrace and Berezinian. Let $\mathcal{A} = \mathcal{A}^0 \oplus \mathcal{A}^1$ be a commutative superalgebra. We have the following general notion of a graded matrix algebra.

Definition. A graded matrix algebra with coefficients in $\mathcal{A}$ is a superalgebra $\mathrm{Mat}_{\mathcal{A}}(p|q)$ of 2×2 block-matrices

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

where A_{11}, A_{12}, A_{21}, and A_{22} are, respectively, matrices of orders $p \times p$, $p \times q$, $q \times p$, and $q \times q$ with elements in $\mathcal{A}$. The element $A \in \mathrm{Mat}_{\mathcal{A}}(p|q)$ is even if corresponding matrices A_{11} and A_{22} consist of even elements of $\mathcal{A}$, and matrices A_{12} and A_{21} consist of odd elements of $\mathcal{A}$. The element $A \in \mathrm{Mat}_{\mathcal{A}}(p|q)$ is odd if matrices A_{11} and A_{22} consist of odd elements of $\mathcal{A}$, and A_{12} and A_{21} consist of even elements of $\mathcal{A}$. The graded vector space $\mathrm{Mat}_{\mathcal{A}}(p|q)$ is a superalgebra with the product given by the matrix multiplication.

The algebra $\mathrm{Mat}(p|q)$ in Example 3.6 corresponds to the case $\mathcal{A} = \mathbb{C}$; another interesting example is when $\mathcal{A}$ is a Grassmann algebra.

It is quite remarkable that such basic notions of linear algebra as trace and determinant admit non-trivial generalizations for graded matrix algebras.

Definition. A supertrace on a graded matrix algebra is a linear mapping $\mathrm{Tr}_s : \mathrm{Mat}_{\mathcal{A}}(p|q) \to \mathcal{A}$, defined by

$$\mathrm{Tr}_s A = \mathrm{Tr}\, A_{11} - (-1)^{|A|}\,\mathrm{Tr}\, A_{22}, \quad A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \in \mathrm{Mat}_{\mathcal{A}}(p|q)$$

where Tr is the ordinary matrix trace.

Proposition 3.1 (The cyclic property of the supertrace).

$$\mathrm{Tr}_s AB = (-1)^{|A||B|}\,\mathrm{Tr}_s BA, \quad A, B \in \mathrm{Mat}_{\mathcal{A}}(p|q).$$

Proof. We check only the case when both 2×2 block-matrices A and B are even elements of $\mathrm{Mat}_{\mathcal{A}}(p|q)$. Other cases are treated similarly and are left to the reader. We have, using the cyclic property of the trace,

$$\begin{aligned} \mathrm{Tr}_s AB &= \mathrm{Tr}\,(A_{11}B_{11} + A_{12}B_{21}) - \mathrm{Tr}\,(A_{21}B_{12} + A_{22}B_{22}) \\ &= \mathrm{Tr}\,(B_{11}A_{11} - B_{21}A_{12}) - \mathrm{Tr}\,(-B_{12}A_{21} + B_{22}A_{22}) = \mathrm{Tr}_s BA. \end{aligned}$$

The superalgebra $\mathrm{End}\,(\mathscr{H}_F)$ corresponds to the case $\mathcal{A} = \mathbb{C}$ and is isomorphic to $\mathrm{Mat}\,(2^{n-1}|2^{n-1})$. The supertace on $\mathrm{End}\,(\mathscr{H}_F)$ is given by

$$\mathrm{Tr}_s\, A = \mathrm{Tr}\, A_{11} - \mathrm{Tr}\, A_{22} = \mathrm{Tr}\, A\Gamma, \quad A \in \mathrm{End}\,(\mathscr{H}_F)\,, \tag{3.2}$$

where Γ is the chirality operator (see Section 1.2). It has the following 2×2 block-matrix form:

$$\Gamma = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix},$$

where I stands for the identity operator in $\mathscr{H}_F^0$ and $\mathscr{H}_F^1$.
It is a non-trivial problem to define a superdeterminant - a natural analog of the determinant for graded matrix algebras, which is multiplicative and generalizes the rule $\det e^A = e^{\mathrm{Tr}\, A}$. The corresponding notion, which is defined only for invertible $A \in \mathrm{Mat}_{\mathcal{A}}(p|q)$, was introduced by F.A. Berezin. It is now commonly called Berezinian and is denoted by $\mathrm{Ber}(A)$.

Consider first the case of even diagonal $A = \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix}$. The relation

$$\mathrm{Ber}\left(e^A\right) = e^{\mathrm{Tr}_s\, A}$$

defines the Berezinian by

$$\mathrm{Ber}(A) = \det A_{11} \det A_{22}^{-1}.$$

Thus in this case the even $q \times q$ matrix A_{22} is necessarily invertible, i.e., $\det A_{22}$ is an invertible element of the commutative algebra $\mathcal{A}^0$, so that the inverse matrix A_{22}^{-1} exists. Now consider the general even $A \in \mathrm{Mat}_{\mathcal{A}}(p|q)$, and suppose that A_{22} is invertible. It is easy to verify the following analog of the Gauss decomposition:

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} I_p & A_{12}A_{22}^{-1} \\ 0 & I_q \end{pmatrix} \begin{pmatrix} A_{11} - A_{12}A_{22}^{-1}A_{21} & 0 \\ 0 & A_{22} \end{pmatrix} \begin{pmatrix} I_p & 0 \\ A_{22}^{-1}A_{21} & I_q \end{pmatrix},$$

where I_p and I_q are, respectively $p \times p$ and $q \times q$ identity matrices. This justifies the following definition.

Definition. Let $A \in \mathrm{Mat}_{\mathcal{A}}(p|q)$ be even and such that the corresponding even $q \times q$ matrix A_{22} is invertible. Then the Berezinian (superdeterminant) of A is given by

$$\mathrm{Ber}(A) = \det\left(A_{11} - A_{12}A_{22}^{-1}A_{21}\right) \det A_{22}^{-1}.$$

Assuming that the $p \times p$ matrix A_{11} is invertible, we get the decomposition

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} I_p & 0 \\ A_{21}A_{11}^{-1} & I_q \end{pmatrix} \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} - A_{21}A_{11}^{-1}A_{12} \end{pmatrix} \begin{pmatrix} I_p & A_{11}^{-1}A_{12} \\ 0 & I_q \end{pmatrix},$$

which suggests that also

$$\mathrm{Ber}(A) = \det A_{11} \det\left(A_{22} - A_{21}A_{11}^{-1}A_{12}\right)^{-1}.$$

It is a fundamental fact that for even invertible $A \in \mathrm{Mat}_{\mathcal{A}}(p|q)$ these two formulas for the Berezinian coincide.

Theorem 3.1. Let

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

be an even element of $\mathrm{Mat}_{\mathcal{A}}(p|q)$. Then
(i) A is invertible if and only if the matrices A_{11} and A_{22} are invertible.
(ii) For invertible $A, \mathrm{Ber}(A)$ is an invertible element of $\mathcal{A}^0$ satisfying
$\mathrm{Ber}(A) = \det\left(A_{11} - A_{12}A_{22}^{-1}A_{21}\right)\det A_{22}^{-1} = \det A_{11}\det\left(A_{22} - A_{21}A_{11}^{-1}A_{12}\right)^{-1}$ and

$$\mathrm{Ber}\left(A^{-1}\right) = \mathrm{Ber}(A)^{-1}$$

(iii) If even $A, B \in \mathrm{Mat}_{\mathcal{A}}(p|q)$ are invertible, then

$$\mathrm{Ber}(AB) = \mathrm{Ber}(A)\,\mathrm{Ber}(B)$$

Problem 3.

5. Complete the proof of Proposition 3.1.

Problem 3.

6. Prove Theorem 3.1.

4.4.4 4. Path Integrals for Anticommuting Variables

4.1. Wick and matrix symbols.

Here we describe the calculus of Wick and matrix symbols of operators in the fermion Hilbert space $\mathscr{H}_F$, which is analogous to the treatment of Wick and matrix symbols in the holomorphic representation in Section 2.7 of Chapter 2. As well as in the bosonic case, it is a tradition to work in anti-holomorphic representation by using $\mathscr{H}_F = \mathbb{C}\left[\bar{\theta}_1, ..., \bar{\theta}_n\right]$ as the fermion Hilbert space with the annihilation and creation operators

$$a_k = \hat{\bar{\theta}}_k \quad \text{and} \quad a_k^* = \frac{\partial}{\partial\bar{\theta}_k}, \quad k = 1, ..., n \tag{4.1}$$

The inner product (2.11) takes the form

$$(f_1, f_2) = \int f_1(\overline{\boldsymbol{\theta}})\overline{f_2(\overline{\boldsymbol{\theta}})}e^{-\boldsymbol{\theta}\overline{\boldsymbol{\theta}}}d\overline{\boldsymbol{\theta}}d\boldsymbol{\theta} \tag{4.2}$$

and the monomials

$$f_I(\overline{\boldsymbol{\theta}}) = \bar{\theta}_{i_1}...\bar{\theta}_{i_k}, \quad 1 \le i_1 < \cdots < i_k \le n$$

parametrized by subsets $I = \{i_1, ..., i_k\} \subseteq \{1, ..., n\}$, form an orthonormal basis in $\mathscr{H}_F$.

Definition. A matrix symbol of an operator $A : \mathscr{H}_F \to \mathscr{H}_F$ is an element $\tilde{A}(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}) \in \mathbb{C}\left[\bar{\theta}_1, ..., \bar{\theta}_n, \theta_1, ..., \theta_n\right]$, defined by

$$\begin{aligned}\tilde{A}(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}) &= \sum_{I,J}(Af_J, f_I)\, f_I(\overline{\boldsymbol{\theta}})\overline{f_J(\overline{\boldsymbol{\theta}})} \\ &= \sum_{I,J}(Af_J, f_I)\,\bar{\theta}_{i_1}...\bar{\theta}_{i_k}\theta_{j_l}...\theta_{j_1}\end{aligned}$$

Here summation goes over all subsets $I = \{i_1, ..., i_k\}$ and $J = \{j_1, ..., j_l\}$ of the set $\{1, ..., n\}$, and as in Section 2.3, we denote by $\overline{f(\overline{\boldsymbol{\theta}})}$ a natural involution on the Grassmann algebra $\mathbb{C}\left[\bar{\theta}_1, ..., \bar{\theta}_n, \theta_1, ..., \theta_n\right]$,

$$\overline{f_J(\overline{\boldsymbol{\theta}})} = \theta_{j_l}...\theta_{j_1} \quad \text{for} \quad f_J(\overline{\boldsymbol{\theta}}) = \bar{\theta}_{j_1}...\bar{\theta}_{j_l}.$$

According to Proposition 1.1, $C_{2n} \simeq \mathrm{End}\,(\mathscr{H}_F)$, so that every operator $A : \mathscr{H}_F \to \mathscr{H}_F$ can be uniquely represented in a Wick normal form as follows:

$$A = \sum_{I,J} K_{IJ} a^*_{i_1}...a^*_{i_k} a_{j_1}...a_{j_l}.$$

Definition. A Wick symbol of an operator $A : \mathscr{H}_F \to \mathscr{H}_F$ is an element $A(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}) \in \mathbb{C}\left[\bar{\theta}_1, ..., \bar{\theta}_n, \theta_1, ..., \theta_n\right]$, defined by

$$A(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}) = \sum_{I,J} K_{IJ} \bar{\theta}_{i_1}...\bar{\theta}_{i_k} \theta_{j_1}...\theta_{j_l}$$

Remark. The definition of matrix and Wick symbols in the fermion case repeats verbatim the corresponding definition for the bosonic case in Section 2.7 of Chapter 2. Note, however, that in the fermion case the product $\theta_{j_l}...\theta_{j_1}$ in the definition of the matrix symbol has reverse ordering, as is required by the inner product (4.2) in $\mathbb{C}\left[\bar{\theta}_1, ..., \bar{\theta}_n\right]$.

To matrix and Wick symbols $\tilde{A}(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta})$ and $A(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta})$ of an operator A one canonically associates elements $\tilde{A}(\overline{\boldsymbol{\theta}}, \boldsymbol{\alpha}), A(\overline{\boldsymbol{\theta}}, \boldsymbol{\alpha})$ and $\tilde{A}(\overline{\boldsymbol{\alpha}}, \boldsymbol{\theta}), A(\overline{\boldsymbol{\alpha}}, \boldsymbol{\theta})$ in the larger Grassmann algebra

$$\mathbb{C}[\boldsymbol{\alpha}, \overline{\boldsymbol{\alpha}}, \boldsymbol{\theta}, \overline{\boldsymbol{\theta}}] = \mathbb{C}\left[\alpha_1, ..., \alpha_n, \bar{\alpha}_1, ..., \bar{\alpha}_n, \theta_1, ..., \theta_n \bar{\theta}_1, ..., \bar{\theta}_n\right]$$

by replacing, correspondingly, θ_i by α_i and $\bar{\theta}_i$ by $\bar{\alpha}_i$. The incomplete Berezin integral $\int d\boldsymbol{\alpha} d\overline{\boldsymbol{\alpha}}$ on $\mathbb{C}[\boldsymbol{\alpha}, \overline{\boldsymbol{\alpha}}, \boldsymbol{\theta}, \overline{\boldsymbol{\theta}}]$ is defined by

$$\int f d\boldsymbol{\alpha} d\overline{\boldsymbol{\alpha}} = \frac{\partial}{\partial \bar{\alpha}_n} \frac{\partial}{\partial \alpha_n} \cdots \frac{\partial}{\partial \bar{\alpha}_1} \frac{\partial}{\partial \alpha_1} f, \quad f \in \mathbb{C}[\boldsymbol{\alpha}, \overline{\boldsymbol{\alpha}}, \boldsymbol{\theta}, \overline{\boldsymbol{\theta}}],$$

and has the property

$$\int h(\boldsymbol{\theta}, \overline{\boldsymbol{\theta}}) g(\boldsymbol{\alpha}, \overline{\boldsymbol{\alpha}}) d\boldsymbol{\alpha} d\overline{\boldsymbol{\alpha}} = h(\boldsymbol{\theta}, \overline{\boldsymbol{\theta}}) \int g(\boldsymbol{\alpha}, \overline{\boldsymbol{\alpha}}) d\boldsymbol{\alpha} d\overline{\boldsymbol{\alpha}} \tag{4.3}$$

We will also use the incomplete Berezin integral $\int d\overline{\boldsymbol{\theta}} d\boldsymbol{\theta}$, defined by

$$\int f d\overline{\boldsymbol{\theta}} d\boldsymbol{\theta} = \frac{\partial}{\partial \theta_n} \frac{\partial}{\partial \bar{\theta}_n} \cdots \frac{\partial}{\partial \theta_1} \frac{\partial}{\partial \bar{\theta}_1} f, \quad f \in \mathbb{C}[\boldsymbol{\alpha}, \overline{\boldsymbol{\alpha}}, \boldsymbol{\theta}, \overline{\boldsymbol{\theta}}].$$

As follows from the proof of Corollary 2.1,

$$\int (a^*_k f_1)\, \overline{f_2} e^{-\boldsymbol{\theta}\overline{\boldsymbol{\theta}}} d\overline{\boldsymbol{\theta}} d\boldsymbol{\theta} = -(-1)^{|f|_1 + |f_2|} \int f_1 \overline{(a_k f_2)} e^{-\boldsymbol{\theta}\overline{\boldsymbol{\theta}}} d\overline{\boldsymbol{\theta}} d\boldsymbol{\theta} \tag{4.4}$$

where operators a^*_k and a_k are given by (4.1), and $f_1, f_2 \in \mathbb{C}[\boldsymbol{\alpha}, \overline{\boldsymbol{\alpha}}, \boldsymbol{\theta}, \overline{\boldsymbol{\theta}}]$.
The next result shows that the matrix symbol of an operator A in $\mathscr{H}_F$, which is just a $2^n \times 2^n$ matrix, can be considered as an integral kernel in anticommuting variables!

Lemma 4.1. Let $\tilde{A}(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta})$ be the matrix symbol of an operator A in $\mathscr{H}_F$. Then for every $f(\overline{\boldsymbol{\theta}}) \in \mathscr{H}_F$,

$$(Af)(\overline{\boldsymbol{\theta}}) = \int \tilde{A}(\overline{\boldsymbol{\theta}}, \boldsymbol{\alpha}) f(\overline{\boldsymbol{\alpha}}) e^{-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}} d\boldsymbol{\alpha} d\overline{\boldsymbol{\alpha}} \tag{4.5}$$

Proof. It is sufficient to verify (4.5) for $f = f_K$, where $K = \{k_1, ..., k_m\} \subseteq \{1, ..., n\}$. Using (4.3) and Lemma 2.5, we get

$$\int \tilde{A}(\overline{\boldsymbol{\theta}},\boldsymbol{\alpha})f_K(\overline{\boldsymbol{\alpha}})e^{-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}}d\boldsymbol{\alpha}d\overline{\boldsymbol{\alpha}} = \sum_{I,J}\left(Af_J,f_I\right)f_I(\overline{\boldsymbol{\theta}})\int \overline{f_J(\overline{\boldsymbol{\alpha}})}f_K(\overline{\boldsymbol{\alpha}})e^{-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}}d\boldsymbol{\alpha}d\overline{\boldsymbol{\alpha}}$$
$$= \sum_{I}\left(Af_K,f_I\right)f_I(\overline{\boldsymbol{\theta}}) = \left(Af_K\right)(\overline{\boldsymbol{\theta}})$$

Next, we introduce Grassmann analogs of the coherent states (see Section 2.7 of Chapter 2). Put

$$\Phi_{\boldsymbol{\alpha}}(\overline{\boldsymbol{\theta}}) = e^{\overline{\boldsymbol{\theta}}\boldsymbol{\alpha}} = \sum_I f_I(\overline{\boldsymbol{\theta}})\overline{f_I(\overline{\boldsymbol{\alpha}})} \quad \text{and} \quad \tilde{\Phi}_{\boldsymbol{\alpha}}(\boldsymbol{\theta}) = e^{-\overline{\boldsymbol{\theta}}\boldsymbol{\alpha}} = \sum_I \overline{f_I(\overline{\boldsymbol{\alpha}})}f_I(\overline{\boldsymbol{\theta}})$$

As in the bosonic case, elements $\Phi_{\boldsymbol{\alpha}}, \tilde{\Phi}_{\boldsymbol{\alpha}} \in \mathbb{C}[\boldsymbol{\alpha},\overline{\boldsymbol{\alpha}},\boldsymbol{\theta},\overline{\boldsymbol{\theta}}]$ satisfy

$$a_k\Phi_{\boldsymbol{\alpha}} = \alpha_k\Phi_{\boldsymbol{\alpha}} \quad \text{and} \quad a_k\tilde{\Phi}_{\boldsymbol{\alpha}} = -\alpha_k\tilde{\Phi}_{\boldsymbol{\alpha}}, \quad k = 1,...,n \tag{4.6}$$

It is very easy to express the matrix symbol of an operator in terms of the coherent states.

Lemma 4.2. Let $\tilde{A}(\overline{\boldsymbol{\alpha}},\boldsymbol{\alpha})$ be the matrix symbol of an operator A in $\mathscr{H}_F$. Then

$$\tilde{A}(\overline{\boldsymbol{\alpha}},\boldsymbol{\alpha}) = \left(A\Phi_{\boldsymbol{\alpha}},\tilde{\Phi}_{\boldsymbol{\alpha}}\right)$$

Proof. The proof is a straightforward computation (cf. the proof of Lemma 2.4 in Section 2.7 of Chapter 2):

$$\tilde{A}(\overline{\boldsymbol{\alpha}},\boldsymbol{\alpha}) = \sum_{I,J}\left(Af_J,f_I\right)f_I(\overline{\boldsymbol{\alpha}})\overline{f_J(\overline{\boldsymbol{\alpha}})}$$
$$= \sum_{I,J}\left(Af_J\overline{f_J(\overline{\boldsymbol{\alpha}})},\overline{f_I(\overline{\boldsymbol{\alpha}})}f_I\right) = \left(A\Phi_{\boldsymbol{\alpha}},\tilde{\Phi}_{\boldsymbol{\alpha}}\right)$$

The next result is an exact analog of Lemma 2.4 in Section 2.7 of Chapter 2.

Lemma 4.3. The matrix and Wick symbols of an operator A in $\mathscr{H}_F$ are related by

$$\tilde{A}(\overline{\boldsymbol{\alpha}},\boldsymbol{\alpha}) = e^{\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}}A(\overline{\boldsymbol{\alpha}},\boldsymbol{\alpha})$$

Moreover, $\tilde{A}(\overline{\boldsymbol{\alpha}},\boldsymbol{\theta}) = e^{\overline{\boldsymbol{\alpha}}\boldsymbol{\theta}}A(\overline{\boldsymbol{\alpha}},\boldsymbol{\theta})$ and $\tilde{A}(\overline{\boldsymbol{\theta}},\boldsymbol{\alpha}) = e^{\overline{\boldsymbol{\theta}}\boldsymbol{\alpha}}A(\overline{\boldsymbol{\theta}},\boldsymbol{\alpha})$.

Proof. As follows from the definition of coherent states,

$$\left(\Phi_{\boldsymbol{\alpha}},\tilde{\Phi}_{\boldsymbol{\alpha}}\right) = e^{\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}}$$

Now representing the operator A in a Wick normal form and using properties (4.4) and (4.6), we obtain

$$\left(A\Phi_{\boldsymbol{\alpha}},\tilde{\Phi}_{\boldsymbol{\alpha}}\right) = \sum_{I,J}K_{IJ}\left(a^*_{i_1}...a^*_{i_k}a_{j_1}...a_{j_l}\Phi_{\boldsymbol{\alpha}},\tilde{\Phi}_{\boldsymbol{\alpha}}\right)$$
$$= \sum_{I,J}(-1)^{kl+k}K_{IJ}\left(a_{j_1}...a_{j_l}\Phi_{\boldsymbol{\alpha}},a_{i_k}...a_{i_1}\tilde{\Phi}_{\boldsymbol{\alpha}}\right)$$
$$= \sum_{I,J}(-1)^{kl}K_{IJ}\left(\alpha_{j_1}...\alpha_{j_l}\Phi_{\boldsymbol{\alpha}},\alpha_{i_k}...\alpha_{i_1}\tilde{\Phi}_{\boldsymbol{\alpha}}\right)$$
$$= \sum_{I,J}(-1)^{kl}K_{IJ}\alpha_{j_1}...\alpha_{j_l}\bar{\alpha}_{i_1}...\bar{\alpha}_{i_k}\left(\Phi_{\boldsymbol{\alpha}},\tilde{\Phi}_{\boldsymbol{\alpha}}\right)$$
$$= A(\overline{\boldsymbol{\alpha}},\boldsymbol{\alpha})\left(\Phi_{\boldsymbol{\alpha}},\tilde{\Phi}_{\boldsymbol{\alpha}}\right) = e^{\overline{\boldsymbol{\alpha}\alpha}}A(\overline{\boldsymbol{\alpha}},\boldsymbol{\alpha})$$

The same computation, after replacing $\Phi_{\boldsymbol{\alpha}}$ by Φ_θ, or $\tilde{\Phi}_{\boldsymbol{\alpha}}$ by $\tilde{\Phi}_\theta$, proves the remaining two formulas.

Thus we have shown that $2^n \times 2^n$ matrices - operators in the fermion Hilbert space $\mathscr{H}_F$ - can be considered as integral operators in anticommuting variables with the integral kernels given by matrix or Wick symbols. The next result is an exact analog of Theorem 2.2 in Section 2.7 of Chapter 2, and establishes the calculus of symbols for operators in $\mathscr{H}_F$.

Theorem 4.1. Let A_1 and A_2 be operators in $\mathscr{H}_F$ with matrix symbols $\tilde{A}_1(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta})$ and $\tilde{A}_2(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta})$ and Wick symbols $A_1(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta})$ and $A_2(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta})$. Then the following formulas hold.
(i) The matrix and Wick symbols of the operator $A = A_1 A_2$ are given by

$$\tilde{A}(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}) = \int \tilde{A}_1(\overline{\boldsymbol{\theta}}, \boldsymbol{\alpha}) \tilde{A}_2(\overline{\boldsymbol{\alpha}}, \boldsymbol{\theta}) e^{-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}} d\boldsymbol{\alpha} d\overline{\boldsymbol{\alpha}}$$

$$A(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}) = \int A_1(\overline{\boldsymbol{\theta}}, \boldsymbol{\alpha}) A_2(\overline{\boldsymbol{\alpha}}, \boldsymbol{\theta}) e^{-(\overline{\boldsymbol{\theta}} - \overline{\boldsymbol{\alpha}})(\boldsymbol{\theta} - \boldsymbol{\alpha})} d\boldsymbol{\alpha} d\overline{\boldsymbol{\alpha}}$$

(ii) The trace and supertrace of an operator A in $\mathscr{H}_F$ are given by

$$\operatorname{Tr} A = \int \tilde{A}(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}) e^{-\boldsymbol{\theta}\overline{\boldsymbol{\theta}}} d\overline{\boldsymbol{\theta}} d\boldsymbol{\theta} = \int A(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}) e^{-2\boldsymbol{\theta}\overline{\boldsymbol{\theta}}} d\overline{\boldsymbol{\theta}} d\boldsymbol{\theta}$$

$$\operatorname{Tr}_s A = \int \tilde{A}(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}) e^{-\overline{\boldsymbol{\theta}}\boldsymbol{\theta}} d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} = \int A(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}) d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}}$$

Proof. Part (i) for matrix symbols is proved by the following straightforward computation:

$$\begin{aligned}
&\int \tilde{A}_1(\overline{\boldsymbol{\theta}}, \boldsymbol{\alpha}) \tilde{A}_2(\overline{\boldsymbol{\alpha}}, \boldsymbol{\theta}) e^{-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}} d\boldsymbol{\alpha} d\overline{\boldsymbol{\alpha}} \\
&= \sum_{I,J} \sum_{K,L} (A_1 f_J, f_I) (A_2 f_L, f_K) \int f_I(\overline{\boldsymbol{\theta}}) \overline{f_J(\overline{\boldsymbol{\alpha}})} f_K(\overline{\boldsymbol{\alpha}}) \overline{f_L(\overline{\boldsymbol{\theta}})} e^{-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}} d\boldsymbol{\alpha} d\overline{\boldsymbol{\alpha}} \\
&= \sum_{I,J,L} (A_1 f_J, f_I) (A_2 f_L, f_J) f_I(\overline{\boldsymbol{\theta}}) \overline{f_L(\overline{\boldsymbol{\theta}})} \\
&= \sum_{I,J,L} (A_2 f_L, f_J) (f_J, A_1^* f_I) f_I(\overline{\boldsymbol{\theta}}) \overline{f_L(\overline{\boldsymbol{\theta}})} \\
&= \sum_{I,L} (A_2 f_L, A_1^* f_I) f_I(\overline{\boldsymbol{\theta}}) \overline{f_L(\overline{\boldsymbol{\theta}})} = \sum_{I,L} (A_1 A_2 f_L, f_I) f_I(\overline{\boldsymbol{\theta}}) \overline{f_L(\overline{\boldsymbol{\theta}})} \\
&= \tilde{A}(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta})
\end{aligned}$$

The corresponding formula for the Wick symbols now follows from Lemma 4.3. The proof of part (ii) is also straightforward. We have

$$\begin{aligned}
\int \tilde{A}(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}) e^{-\boldsymbol{\theta}\overline{\boldsymbol{\theta}}} d\overline{\boldsymbol{\theta}} d\boldsymbol{\theta} &= \sum_{I,J} (A f_J, f_I) \int f_I(\overline{\boldsymbol{\theta}}) \overline{f_J(\overline{\boldsymbol{\theta}})} e^{-\boldsymbol{\theta}\overline{\boldsymbol{\theta}}} d\overline{\boldsymbol{\theta}} d\boldsymbol{\theta} \\
&= \sum_I (A f_I, f_I) = \operatorname{Tr} A
\end{aligned}$$

Similarly,

$$\begin{aligned}
\int \tilde{A}(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}) e^{-\overline{\boldsymbol{\theta}}\boldsymbol{\theta}} d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} &= \sum_{I,J} (A f_J, f_I) \int f_I(\overline{\boldsymbol{\theta}}) \overline{f_J(\overline{\boldsymbol{\theta}})} e^{-\overline{\boldsymbol{\theta}}\boldsymbol{\theta}} d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} \\
&= \sum_I (-1)^{|I|} (A f_I, f_I) = \operatorname{Tr}_s A
\end{aligned}$$

where $|I|$ denotes the cardinality of the subset $I \subseteq \{1, ..., n\}$. Corresponding formulas for the Wick symbol follow from Lemma 4.3.

Problem 4.1. Verify directly all results in this section for the simplest case of one degree of freedom, when $\mathscr{H}_F = \mathbb{C}^2$.

Problem 4.2. Show that the Wick symbol of the product $A = A_l ... A_1$ is given by

$$A(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}) = \int \cdots \int A_l \left(\overline{\boldsymbol{\theta}}, \boldsymbol{\alpha}_{l-1}\right) ... A_1 \left(\overline{\boldsymbol{\alpha}}_1, \boldsymbol{\theta}\right) \exp\left\{\sum_{k=1}^{l-1} \overline{\boldsymbol{\alpha}}_k \left(\boldsymbol{\alpha}_{k-1} - \boldsymbol{\alpha}_k\right) + \overline{\boldsymbol{\theta}} \left(\boldsymbol{\alpha}_{l-1} - \boldsymbol{\theta}\right)\right\}$$
$$d\boldsymbol{\alpha}_1 d\overline{\boldsymbol{\alpha}}_1 ... d\boldsymbol{\alpha}_{l-1} d\overline{\boldsymbol{\alpha}}_{l-1}$$

where $\boldsymbol{\alpha}_0 = \boldsymbol{\theta}$ and $A_k(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta})$ are the Wick symbols of the operators A_k.

Problem 4.3. Prove that the Wick symbol $\Gamma(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta})$ of the chirality operator Γ is $e^{-2\bar{\theta}\theta}$.

4.2. Path integral for the evolution operator. Let H be a Hamiltonian of a system of n fermions - an operator in $\mathscr{H}_F$ with the Wick symbol $H(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta})$. Here we express the Wick symbol $U(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}; T)$ of the evolution operator $U(T) = e^{-iTH}$ by using the path integral over Grassmann variables. Our exposition will be parallel to that in Section 2.4 of Chapter 5, with obvious simplification due to the fact that fermion Hilbert space $\mathscr{H}_F$ is finitedimensional. Namely, the following elementary result replaces assumption (2.11), made in Section 2.4 of Chapter 5.

Lemma 4.4. Let $\tilde{U}(\Delta t)$ be the operator with the Wick symbol $e^{-iH(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta})\Delta t}$. Then

$$U(T) = \lim_{N \to \infty} \tilde{U}(\Delta t)^N, \quad \text{where} \quad \Delta t = \frac{T}{N}.$$

Proof. The Wick symbol of the operator $R(\Delta t) = I - i\hat{H}\Delta t - \tilde{U}(\Delta t)$ is a polynomial in Δt with Grassmann algebra coefficients, which starts with the term $(\Delta t)^2$. It is easy to see that $\|R(\Delta t)\| \leq c(\Delta t)^2$ for some $c > 0$, and

$$U(T) = \lim_{N \to \infty} (I - iH\Delta t)^N = \lim_{N \to \infty} (U(\Delta t) + R(\Delta t))^N = \lim_{N \to \infty} \tilde{U}(\Delta t)^N$$

Using the formula for the composition of Wick symbols (see Theorem 4.1 and Problem 4.2), we can represent the Wick symbol $U_N(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}; T)$ of the operator $\tilde{U}(\Delta t)^N$ as an $(N-1)$-fold Berezin integral. Namely, consider the anticommuting variables $\boldsymbol{\alpha}_k = \{\alpha_k^1, ..., \alpha_k^n\}, \overline{\boldsymbol{\alpha}}_k = \{\bar{\alpha}_k^1, ..., \bar{\alpha}_k^n\}, k = 1, ..., N-1$ - generators of the Grassmann algebra with involution – and denote $\overline{\boldsymbol{\alpha}}_k \boldsymbol{\alpha}_k = \sum_{l=1}^n \bar{\alpha}_k^l \alpha_k^l$, etc. Then

$$U_N(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}; T) = \int \cdots \int \exp\left\{\sum_{k=1}^{N} \left(\overline{\boldsymbol{\alpha}}_k \left(\boldsymbol{\alpha}_{k-1} - \boldsymbol{\alpha}_k\right) + \overline{\boldsymbol{\theta}} \left(\boldsymbol{\alpha}_N - \boldsymbol{\theta}\right)\right.\right.$$
$$\left.\left. -iH\left(\overline{\boldsymbol{\alpha}}_k, \boldsymbol{\alpha}_{k-1}\right)\Delta t\right)\right\} \prod_{k=1}^{N-1} d\boldsymbol{\alpha}_k d\overline{\boldsymbol{\alpha}}_k$$

where $\boldsymbol{\alpha}_0 = \boldsymbol{\theta}$, and we put $\overline{\boldsymbol{\alpha}}_N = \overline{\boldsymbol{\theta}}$. It follows from Lemma 4.4 that

$$U(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}; T) = \lim_{N \to \infty} U_N(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}; T) = \lim_{N \to \infty} \int \cdots \int \tag{4.7}$$

$$\exp\left\{\sum_{k=1}^{N} \left(\overline{\boldsymbol{\alpha}}_k \left(\boldsymbol{\alpha}_{k-1} - \boldsymbol{\alpha}_k\right) + \overline{\boldsymbol{\theta}} \left(\boldsymbol{\alpha}_N - \theta\right) - iH\left(\overline{\boldsymbol{\alpha}}_k, \boldsymbol{\alpha}_{k-1}\right)\Delta t\right)\right\} \prod_{k=1}^{N-1} d\boldsymbol{\alpha}_k d\overline{\boldsymbol{\alpha}}_k$$

This formula looks exactly the same as the corresponding formula (2.13) for the Wick symbol of the evolution operator in Section 2.4 of Chapter 5! Accordingly, we interpret the

limit $N \to \infty$ as the following Feynman path integral for Grassmann variables (or Grassmann path integral):

$$U(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}; T) = \int_{\substack{\overline{\boldsymbol{\alpha}}(T)=\overline{\boldsymbol{\theta}} \\ \boldsymbol{\alpha}(0)=\boldsymbol{\theta}}} e^{i\int_0^T (i\overline{\boldsymbol{\alpha}}\dot{\boldsymbol{\alpha}} - H(\overline{\boldsymbol{\alpha}},\boldsymbol{\alpha}))dt + \overline{\boldsymbol{\theta}}(\boldsymbol{\alpha}(T)-\boldsymbol{\theta})} \mathscr{D}\boldsymbol{\alpha}\mathscr{D}\overline{\boldsymbol{\alpha}}. \tag{4.8}$$

Here the "integration" goes over all functions $\boldsymbol{\alpha}(t), \overline{\boldsymbol{\alpha}}(t)$ with anticommuting values [2] on the interval $[0, T]$, satisfying boundary conditions $\boldsymbol{\alpha}(0) = \boldsymbol{\theta}$, $\overline{\boldsymbol{\alpha}}(T) = \overline{\boldsymbol{\theta}}$, and

$$\mathscr{D}\boldsymbol{\alpha}\mathscr{D}\overline{\boldsymbol{\alpha}} = \prod_{0\le t\le T} d\boldsymbol{\alpha}(t) d\overline{\boldsymbol{\alpha}}(t) = \lim_{N\to\infty} \prod_{k=1}^{N-1} d\boldsymbol{\alpha}_k d\overline{\boldsymbol{\alpha}}_k.$$

As in Section 2.4 of Chapter 5, for $0 < t < T$ variables $\overline{\boldsymbol{\alpha}}(t)$ are conjugated to $\boldsymbol{\alpha}(t)$ with respect to the Grassmann algebra involution, while $\overline{\boldsymbol{\alpha}}(0)$ and $\boldsymbol{\alpha}(T)$ - also variables of integration - are not conjugated to the boundary values $\boldsymbol{\alpha}(0) = \boldsymbol{\theta}, \overline{\boldsymbol{\alpha}}(T) = \overline{\boldsymbol{\theta}}$.

Remark. It should be emphasized that the only rigorous meaning of the Grassmann path integral (4.8) is the limit of multiple Berezin integrals in (4.7). However, as we have seen already in Chapter 5, it is very useful to pretend that the path integral has an independent definition, and formally work with it as if it was an actual integral.

Using Theorem 4.1, it is easy to express the supertrace of the evolution operator $U(T)$ - an operator in a finite-dimensional Hilbert space $\mathscr{H}_F$ as a Grassmann path integral. We have

$$\begin{aligned}\operatorname{Tr}_s e^{-iTH} &= \lim_{N\to\infty} \int U_N(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}; T) d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} = \lim_{N\to\infty} \int \cdots \int \exp\{\overline{\boldsymbol{\theta}}(\boldsymbol{\alpha}(T) - \boldsymbol{\theta}) \\ &+ \sum_{k=1}^{N} \left(\overline{\boldsymbol{\alpha}}_k (\boldsymbol{\alpha}_{k-1} - \boldsymbol{\alpha}_k) - iH(\overline{\boldsymbol{\alpha}}_k, \boldsymbol{\alpha}_{k-1})\Delta t\right)\Bigg\} \prod_{k=1}^{N-1} d\boldsymbol{\alpha}_k d\overline{\boldsymbol{\alpha}}_k d\boldsymbol{\theta} d\overline{\boldsymbol{\theta}} \\ &= \int_{\substack{\overline{\boldsymbol{\alpha}}(0)=\overline{\boldsymbol{\alpha}}(T) \\ \boldsymbol{\alpha}(0)=\boldsymbol{\alpha}(T)}} e^{i\int_0^T (i\overline{\boldsymbol{\alpha}}\dot{\boldsymbol{\alpha}} - H(\overline{\boldsymbol{\alpha}},\boldsymbol{\alpha}))dt} \mathscr{D}\boldsymbol{\alpha}\mathscr{D}\overline{\boldsymbol{\alpha}}\end{aligned}$$

- a Grassmann path integral with periodic boundary conditions. Here periodic boundary conditions emerge from $\boldsymbol{\alpha}_0 = \boldsymbol{\theta}$ and $\overline{\boldsymbol{\alpha}}_N = \overline{\boldsymbol{\theta}}$ in the same way as in Section 2.4 of Chapter 5. Namely, since $\overline{\boldsymbol{\theta}}$ and $\boldsymbol{\theta}$ are now variables of integration, the identity (2.17) in Section 2.4 of Chapter 5, which is valid in the case of anticommuting variables as well, ensures that $\boldsymbol{\alpha}_N = \boldsymbol{\theta}$ and $\overline{\boldsymbol{\alpha}}_0 = \overline{\boldsymbol{\theta}}$. Denoting by $\boldsymbol{\Lambda}$ the corresponding "Grassmann loop space" - the space of all functions with anticommuting values $\boldsymbol{\alpha}(t)$ and $\overline{\boldsymbol{\alpha}}(t)$ conjugated with respect to the Grassmann algebra involution and satisfying periodic boundary conditions $\boldsymbol{\alpha}(0) = \boldsymbol{\alpha}(T)$ and $\overline{\boldsymbol{\alpha}}(0) = \overline{\boldsymbol{\alpha}}(T)$ - we can rewrite the previous formula as

$$\operatorname{Tr}_s e^{-iTH} = \int_{\boldsymbol{\Lambda}} e^{i\int_0^T (i\overline{\boldsymbol{\alpha}}\dot{\boldsymbol{\alpha}} - H(\overline{\boldsymbol{\alpha}},\boldsymbol{\alpha}))dt} \mathscr{D}\boldsymbol{\alpha}\mathscr{D}\overline{\boldsymbol{\alpha}}$$

Replacing the physical time t by the Euclidean time $-it$ and T by $-iT$, we get the Grassmann integral representation for the Wick symbol of the operator $U(-iT) = e^{-TH}$,

$$U(\overline{\boldsymbol{\theta}}, \boldsymbol{\theta}; -iT) = \int_{\substack{\overline{\boldsymbol{\alpha}}(T)=\overline{\boldsymbol{\theta}} \\ \boldsymbol{\alpha}(0)=\boldsymbol{\theta}}} e^{-\int_0^T (\overline{\boldsymbol{\alpha}}\dot{\boldsymbol{\alpha}} + H(\overline{\boldsymbol{\alpha}},\boldsymbol{\alpha}))dt} \mathscr{D}\boldsymbol{\alpha}\mathscr{D}\overline{\boldsymbol{\alpha}},$$

and for the supertrace,

[02] For every $0 \le t \le T$ there is a copy of the independent Grassmann algebra with generators $\alpha^1(t), ..., \alpha^n(t), \bar{\alpha}^1(t), ..., \bar{\alpha}^n(t)$.

$$\mathrm{Tr}_s\, e^{-TH} = \int_{\boldsymbol{\Lambda}} e^{-\int_0^T (\overline{\boldsymbol{\alpha}}\dot{\boldsymbol{\alpha}} + H(\overline{\boldsymbol{\alpha}},\boldsymbol{\alpha}))dt} \mathscr{D}\boldsymbol{\alpha}\mathscr{D}\overline{\boldsymbol{\alpha}} \tag{4.9}$$

Problem 4.4. Express the matrix symbol of the evolution operator as the Grassmann path integral.

Problem 4.5. Show that

$$\mathrm{Tr}\, e^{-TH} = \int_{\substack{\overline{\boldsymbol{\alpha}}(0)=-\overline{\boldsymbol{\alpha}}(T)\\ \boldsymbol{\alpha}(0)=-\boldsymbol{\alpha}(T)}} e^{-\int_0^T (\overline{\boldsymbol{\alpha}}\dot{\boldsymbol{\alpha}} + H(\bar{\alpha},\boldsymbol{\alpha}))dt} \mathscr{D}\boldsymbol{\alpha}\mathscr{D}\overline{\boldsymbol{\alpha}}$$

- the Grassmann path integral with anti-periodic boundary conditions.

4.3. Gaussian path integrals over Grassmann variables. For simplicity, here we consider only the case $n = 1$. As in Section 5.3 of Chapter 5, for $u(t) \in C^1([0,T],\mathbb{R})$ we put

$$u_0 = \frac{1}{T}\int_0^T u(t)dt \quad \text{and} \quad D = \frac{d}{dt}$$

and consider on the interval $[0,T]$ the first-order differential operator $D+\, u(t)$ with periodic boundary conditions. The following result evaluates the simplest Gaussian path integral for Grassmann variables.

Theorem 4.2. We have

$$\int_\Lambda e^{-\int_0^T (\bar{\alpha}\dot{\alpha} + u(t)\bar{\alpha}\alpha)dt} \mathscr{D}\alpha\mathscr{D}\bar{\alpha} = \det(D + u(t)) = 1 - e^{-u_0 T}.$$

Proof. Using Lemma 2.4, we get

$$\begin{aligned}
&\int_\Lambda e^{-\int_0^T (\bar{\alpha}\dot{\alpha} + u(t)\bar{\alpha}\alpha)dt} \mathscr{D}\alpha\mathscr{D}\bar{\alpha} \\
&= \lim_{N\to\infty} \int\cdots\int e^{\sum_{k=1}^N (\bar{\alpha}_k(\alpha_{k-1}-\alpha_k) - u(t_k)\bar{\alpha}_k\alpha_{k-1}\Delta t)} \prod_{k=1}^N d\alpha_k d\bar{\alpha}_k \\
&= \lim_{N\to\infty} \det A_N
\end{aligned}$$

Here $\alpha_0 = \alpha_N, \bar{\alpha}_0 = \bar{\alpha}_N, t_k = k\Delta t$, and A_N is the following $N \times N$ matrix:

$$A_N = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & b_N \\ b_1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & b_2 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & \cdots & b_{N-1} & 1 \end{pmatrix},$$

where $b_k = -1 + u\,(t_k)\,\Delta t$. We have

$$\det A_N = 1 - (-1)^N \prod_{k=1}^N b_k = 1 - \prod_{k=1}^N (1 - u\,(t_k)\,\Delta t)$$

so that

$$\lim \det A_N = 1 - e^{-\int_0^T u(t)dt} = 1 - e^{-u_0 T}$$

Using Proposition 5.3 in Section 5.3 of Chapter 5 completes the proof.

Example 4.1 (The fermion harmonic oscillator). The fermion analog of the harmonic oscillator is the Hamiltonian

$$H = \frac{1}{2}\omega\left(a^*a - aa^*\right) = \omega\left(a^*a - \frac{1}{2}I\right) = \omega\left(N - \frac{1}{2}I\right),$$

where a^* and a are creation and annihilation operators in the one fermion Hilbert space $\mathscr{H}_F = \mathbb{C}^2$ (see Section 1.1). The Wick symbol H is $H(\bar{\alpha}, \alpha) = \omega\left(\bar{\alpha}\alpha - \frac{1}{2}\right)$. Now using (4.9) and Theorem 4.2, we obtain

$$\begin{aligned}\operatorname{Tr}_s e^{-TH} &= \int_\Lambda e^{-\int_0^T (\bar{\alpha}\dot{\alpha} + H(\bar{\alpha},\alpha))dt}\mathscr{D}\alpha\mathscr{D}\bar{\alpha} \\ &= e^{\frac{\omega T}{2}}\int_\Lambda e^{-\int_0^T(\bar{\alpha}\dot{\alpha}+\omega\bar{\alpha}\alpha)dt}\mathscr{D}\alpha\mathscr{D}\bar{\alpha} = e^{\frac{\omega T}{2}}\left(1 - e^{-\omega T}\right) = 2\sinh\frac{\omega T}{2}.\end{aligned}$$

Of course, the same result can be obtained directly since e^{-TH} is just a 2×2 matrix with eigenvalues $e^{\frac{\omega T}{2}}$ and $e^{-\frac{\omega T}{2}}$ which correspond, respectively, to the eigenspaces $\mathscr{H}_F^0$ and $\mathscr{H}_F^1$. Thus

$$\operatorname{Tr}_s e^{-TH} = e^{\frac{\omega T}{2}} - e^{-\frac{\omega T}{2}} = 2\sinh\frac{\omega T}{2}$$

Remark. We have the following analog of formula (2.6) of Chapter 6 for path integrals over Grassmann variables:

$$\int_\Lambda f(\alpha,\bar{\alpha})\mathscr{D}\alpha\mathscr{D}\bar{\alpha} = \int\left(\int_{\Lambda_0} f(\beta,\theta;\bar{\beta},\bar{\theta})\mathscr{D}\beta\mathscr{D}\bar{\beta}\right)d\theta d\bar{\theta} \tag{4.10}$$

where

$$\alpha(t) = \theta + \beta(t) \quad \text{and} \quad \int_0^T \beta(t)dt = 0$$

and Λ_0 is the space of Grassmann loops $\beta(t), \bar{\beta}(t)$ with zero constant term.

Example 4.2. Using formula (4.10) and Theorem 4.2, we get

$$\begin{aligned}\det(D+\omega) &= \int_\Lambda e^{-\int_0^T(\bar{\alpha}\dot{\alpha}+\omega\bar{\alpha}\alpha)dt}\mathscr{D}\alpha\mathscr{D}\bar{\alpha} \\ &= \int e^{-\omega T\bar{\theta}\theta}d\theta d\bar{\theta}\int_{\Lambda_0} e^{-\int_0^T(\bar{\beta}\dot{\beta}+\omega\bar{\beta}\beta)dt}\mathscr{D}\beta\mathscr{D}\bar{\beta} = \omega T\int_{\Lambda_0} e^{-\int_0^T(\bar{\beta}\dot{\beta}+\omega\bar{\beta}\beta)dt}\mathscr{D}\beta\mathscr{D}\bar{\beta},\end{aligned}$$

so that

$$\int_{\Lambda_0} e^{-\int_0^T \bar{\beta}\dot{\beta}dt}\mathscr{D}\beta\mathscr{D}\bar{\beta} = \lim_{\omega\to 0}\frac{\det(D+\omega)}{\omega T} = \lim_{\omega\to 0}\frac{1-e^{-\omega T}}{\omega T} = 1$$

Equivalently,

$$\int_{\Lambda_0} e^{-\int_0^T \bar{\beta}\dot{\beta}dt}\mathscr{D}\beta\mathscr{D}\bar{\beta} = \frac{1}{T}\det{}' D \tag{4.11}$$

where $\det' D = T$ (see Proposition 5.3 in Section 5.3 of Chapter 5). Introducing

$$\theta_1(t) = \frac{1}{\sqrt{2}}(\beta(t) + \bar{\beta}(t)), \quad \theta_2(t) = \frac{1}{i\sqrt{2}}(\beta(t) - \bar{\beta}(t)),$$

so that $\bar{\theta}_j(t) = \theta_j(t), j = 1, 2$, we can rewrite (4.11) as

$$\int_{\Lambda_0} e^{-\frac{1}{2}\int_0^T (\theta_1\dot\theta_1+\theta_2\dot\theta_2)dt}\mathscr{D}\theta_1\mathscr{D}\theta_2 = \frac{1}{T}\det{}' D = 1$$

Since $\mathrm{Pf}'(D) = \sqrt{\det{}' D} = \sqrt{T}$, we have

$$\int_{\Lambda_0(\mathbb{R})} e^{-\frac{1}{2}\int_0^T \theta\dot\theta dt}\mathscr{D}\theta = \frac{1}{\sqrt{T}}\mathrm{Pf}'(D) = 1. \tag{4.12}$$

Here the domain of integration $\Lambda_0(\mathbb{R})$ consists of all functions $\theta(t)$ with values in the Grassmann algebra over $\mathbb{R}$, which have zero constant term and satisfy periodic boundary conditions $\theta(0) = \theta(T)$. We will use formulas (4.10) and (4.12) in Section 2.2 of Chapter 8.

Problem 4.6. Show that

$$\int_{\substack{\bar\alpha(0)=-\bar\alpha(T)\\ \alpha(0)=-\alpha(T)}} e^{-\int_0^T(\bar\alpha\dot\alpha+u(t)\bar\alpha\alpha)dt}\mathscr{O}\alpha\mathscr{D}\bar\alpha = 1 + e^{-u_0 T}$$

- the regularized determinant of the operator $D+u(t)$ on $[0,T]$ with anti-periodic boundary conditions.

Problem 4.7. For the fermion harmonic oscillator verify that $\mathrm{Tr}\, e^{-TH} = 2\cosh\frac{\omega T}{2}$ directly, and also by using results of Problems 4.5 and 4.6.

Problem 4.8. Prove formula (4.10). (Hint: Follow the proof of Theorem 4.2, and use the decomposition $\alpha_k = \theta + \beta_k$, where $\beta_0 = \beta_N$ and $\sum_{k=1}^N \beta_k = 0$.)

Problem 4.9. Give a direct proof of formula (4.12).

4.5 Spin, Spinors and Identical Particles

Обсудим подробно спин и спиноры.

4.5.1 Operator of Angular Momentum $\hat j$ (!?!!)

(по идее тут вся теория по нему и будет.)

Оператор момента в двух словах

(еще потренировать нужно)

Основные формулы (??)

оператор момента импульса водится как

$$L_x = -i\hbar\partial\phi,$$

что очень схоже с оператором импульса

$$\mathbf{L} = -i[\mathbf{r}\times\boldsymbol{\partial}] = -i\left(\mathbf{e}_\varphi\frac{\partial}{\partial\vartheta} - \mathbf{e}_\theta\frac{1}{\sin\vartheta}\frac{\partial}{\partial\varphi}\right)$$

Можно складывать моменты

(тут укажу коротко эту теорию, подробно - ниже)

Коэффициенты Клебша—Гордана $C^{JM}_{l_1m_1j_2m_2}$, являющиеся коэффициентами векторного сложения, осуществляют разложение приводимых представлений группы вращений на неприводимые.

Все остальные коэффициенты векторного сложения могут быть представлены в виде сумм произведений коэффициентов Клебша—Гордана.

Все это определяет их широкое использование в квантовой теории углового момента.

Суть вывода (??)

(пока суть не так глубоко понял, почему именно такими повышающими, понижающими операторами работаем.)

Обзор применений оператора момента импульса

(вроде в атомах и разных моделях, укажу потом конкретно)

Мы хотим описывать радиальные движения одной частицы вокруг другой, поэтому вводим угловой момент

Вывод оператора момента

И поэтому нам известно, что

$$\left[\hat{\boldsymbol{j}}_\alpha, \hat{\boldsymbol{j}}_\beta\right] = \mathrm{i}\epsilon_{\alpha\beta\gamma}\hat{\boldsymbol{j}}_\gamma; \quad \left[\hat{\boldsymbol{j}}_\alpha, \hat{\boldsymbol{j}}^2\right] = 0; \quad \left[\hat{\boldsymbol{j}}_\alpha, \hat{\boldsymbol{p}}^2\right] = 0; \quad \left[\hat{\boldsymbol{j}}_\alpha, \hat{\boldsymbol{p}}_\beta\right] = \mathrm{i}\epsilon_{\alpha\beta\gamma}\hat{\boldsymbol{p}}_\gamma;$$

Кроме того, если энергия является скаляром, то

$$\left[\hat{\boldsymbol{j}}_\alpha, \hat{H}\right] = 0$$

Составим из взаимнокомутирующих операторов полный набор наблюдаем, например, такой:

$$\hat{H}, \hat{j}^2, \hat{\boldsymbol{p}}^2, \hat{\boldsymbol{j}}_z$$

Действительно, все эти операторы коммутируют, так что они могут быть измерены точно совместно, т.е.

они имеют общие собственные векторы состояния.

Важно подчеркнуть, что компоненты момента импульса, вообще говоря, не могут быть измерены точно совместно, так как их коммутатор не равен нулю.

Исключение составляет случай

$$\hat{\boldsymbol{j}}_\alpha|\Psi\rangle \equiv 0$$

т.е.

если орбитальный и спиновый момент импульса тождествен но равны нулю в данном состояни и.

Рассмотрим задачу на собственные значения к вадрата импульса и одной из его ком по- нент, Для определенности компоненты по оси z:

$$\hat{\boldsymbol{j}}^2|\lambda,\mu\rangle = \lambda|\lambda,\mu\rangle$$
$$\hat{\boldsymbol{j}}_z|\lambda,\mu\rangle = \mu|\lambda,\mu\rangle$$

выполнено условие вырождения: оператор $\hat{\boldsymbol{j}}^2$ коммутирует со всеми компонентами $\boldsymbol{j}$, но эти компоненты не коммутируют друг с другом.

Введем операторы

$$\hat{j}_\pm = \hat{\boldsymbol{j}}_x \pm \mathrm{i}\hat{\boldsymbol{j}}_y, \quad \hat{j}_- = \hat{j}_+^\dagger, \quad \left[\hat{j}_\pm \cdot \hat{\boldsymbol{j}}^2\right] = 0$$

Тогда легко видеть, что

$$\hat{j}_+\hat{j}_- = \hat{j}_x^2 + \hat{j}_y^2 - \mathrm{i}\left(\hat{j}_x\hat{j}_y - \hat{j}_y\hat{j}_x\right) = \hat{j}_x^2 + \hat{j}_y^2 - \mathrm{i}\left[\hat{j}_x, \hat{j}_y\right] = \hat{j}_x^2 + \hat{j}_y^2 + \hat{j}_z$$

и аналогично

$$\hat{j} - \hat{j}_+ = \hat{j}_x^2 + \hat{j}_y^2 - \hat{j}_z$$

В итоге,

$$\hat{\boldsymbol{j}}^2 = \frac{1}{2}\left(\hat{j}_+\hat{j}_- + \hat{j}_-\hat{j}_+\right) + \hat{j}_z^2$$

Коммутатор этих операторов с компонентой $\hat{j}_z$ легко вычисляется

$$\left[\hat{j}_z, \hat{j}_\pm\right] = \left[\hat{j}_z, \hat{j}_x \pm \mathrm{i}\hat{j}_y\right] = \mathrm{i}\hat{j}_y \pm \mathrm{i}\left(-\mathrm{i}\hat{j}_x\right) = \pm\hat{j}_\pm$$

Это позволяет установить, что векторы $\hat{j}_\pm|\lambda,\mu\rangle$ также являются собственным и векторами Заданной пары наблюдаемых:

$$\hat{j}_z\hat{j}_\pm|\lambda,\mu\rangle = \hat{j}_\pm\left(\hat{j}_z \pm 1\right)|\lambda,\mu\rangle = (\mu\pm 1)\hat{j}_\pm|\lambda,\mu\rangle$$

$$\hat{j}_\pm|\lambda,\mu\rangle = \mathcal{N}_\pm(\lambda,\mu)|\lambda,\mu\pm 1\rangle$$

где нормировочные множители $\mathcal{N}_\pm$ легко определить, взяв модуль каждого из состояний:

$$\left\langle\lambda,\mu\left|\hat{j}_-\hat{j}_+\right|\lambda,\mu\right\rangle = \left\langle\lambda,\mu\left|\left(\hat{j}^2 - \hat{j}_z^2 - \hat{j}_z\right)\right|\lambda,\mu\right\rangle = \lambda - \mu^2 - \mu \geqslant 0$$

и аналогично

$$\left\langle\lambda,\mu\left|\hat{j}_+\hat{j}_-\right|\lambda,\mu\right\rangle = \left\langle\lambda,\mu\left|\left(\hat{j}^2 - \hat{j}_z^2 + \hat{j}_z\right)\right|\lambda,\mu\right\rangle = \lambda - \mu^2 + \mu \geqslant 0$$

откуда

$$\hat{j}_\pm|\lambda,\mu\rangle = \sqrt{\lambda - \mu(\mu\pm 1)}|\lambda,\mu\pm 1\rangle$$

Также, как и в случае гармонического осциллятора, использование повышающего и понижающего операторов позволяет провести квантование спектра собственных значений пары $\left\{\hat{\boldsymbol{j}}^2, \hat{j}_z\right\}$ с помощью условия неотрицательности нормы вектора состояния.

В самом деле, повышающий оператор переводит $\mu \to \mu + 1$ и изменяет норм у вектора

$$\mathcal{N}^2 \to \mathcal{N}^2[\lambda - \mu(\mu+1)] \geqslant 0$$

Для того чтобы норма вектора состояния после многократного действия повышающего оператора оставалась положительно определенной, необходимо чтобы цепочка многократного повышения прервалась, т.е. чтобы существовал старший вектор состояния:

$$\hat{j}_+\,|\lambda,\mu_\lambda\rangle = 0, \quad \lambda = \mu_\lambda\,(\mu_\lambda + 1)$$

Составим цепочку состояний, многократно действуя на старший вектор понижающим оператором,

$$|\lambda,\mu_\lambda\rangle\,, \quad \hat{j}_-\,|\lambda,\mu_\lambda\rangle\,, \ldots$$

с собственным и значениям и проекции

$$\mu_\lambda, \quad \mu_\lambda - 1, \ldots$$

Для того чтобы норма векторов в этой цепочке состояний оставалась положительно определенной, необходимо, чтобы она оборвалась, т.е. существовал бы младший вектор:

$$\hat{j}_-\,|\lambda,\nu_\lambda\rangle = 0, \quad \lambda = \nu_\lambda\,(\nu_\lambda - 1)$$

но при этом мы получаем собствен ное значение для младшего вектора путем целого конечного числа шагов из собственного значения для старшего вектора:

$$\nu_\lambda = \mu_\lambda - n, \quad n \in \mathbb{N}$$

Собственное значение λ оператора $\hat{\boldsymbol{j}}^2$ при действии повышающего и понижающего операторов не изменяется (соответствующий ком мутатор равен нулю), так что согласно (8.7), (8.8) имеет место тождество

$$\mu_\lambda\,(\mu_\lambda+1)=(\mu_\lambda-n)\,(\mu_\lambda-n-1)$$

с единствен ным решением

$$\mu_\lambda=\frac{1}{2}n$$

вектора $\mu_\lambda=j$, так что

$$\begin{aligned}\hat{\boldsymbol{j}}^2|j,m\rangle&=j(j+1)|j,m\rangle\\ \hat{j}_z|j,m\rangle&=m|j,m\rangle\\ \hat{j}_+|j,j\rangle&=0\\ \hat{j}_-|j,-j\rangle&=0\end{aligned}$$

причем количество состояний с заданным j равно числу шагов от старшего вектора к младшем у $n=2j$ плюс 1 начальное состояние построения цепочки (старший вектор). т.е. вырождение $\hat{\boldsymbol{j}}^2$ по числу проекций есть

$$k=2j+1$$

где $\{j,m\}$ - полуцелые числа,

$$j=\frac{1}{2}(k-1),\quad k\in\mathbb{N},\quad j\leqslant m\leqslant -j$$

и k -кратность вырождения $\hat{\boldsymbol{j}}^2$. В частности, при $k=1$ имеем $\boldsymbol{j}\equiv 0$.

Кроме того, мы нашли, что матричные элементы повышающего и понижающего операторов задаются формулам и

$$\left\langle j,n\left|\hat{j}_\pm\right|j,m\right\rangle=\sqrt{j(j+1)-m(m\pm1)}\delta_{n,m\pm1}$$

оператор момента в сферических координатах

(выделю потом суть)

Выразим компоненты орбитального момента в полярных координатах.

Например,

$$\hat{l}_z=\boldsymbol{e}_z\cdot\boldsymbol{l}=-\mathrm{i}\boldsymbol{e}_z\cdot[\boldsymbol{r},\boldsymbol{\nabla}]$$

где векторное произведение запишем в полярных координатах

$$[\boldsymbol{r},\boldsymbol{\nabla}]=\boldsymbol{e}_\theta\epsilon_{\theta r\phi}r\frac{\partial}{\partial\ell_\phi}+\boldsymbol{e}_\phi\epsilon_{\phi r\theta}r\frac{\partial}{\partial\ell_\theta}$$

правой тройки базисных векторов

$$\epsilon_{r\theta\phi}=1$$

Отсюда для z -той компоненты находим

$$\hat{l}_z=-\mathrm{i}\frac{\partial}{\partial\phi}$$

Оставшиеся компоненты принимают вид:

$$\begin{aligned}\hat{l}_x&=+\mathrm{i}\sin\phi\frac{\partial}{\partial\theta}+\mathrm{i}\cos\phi\,\mathrm{ctg}\,\theta\frac{\partial}{\partial\phi}\\ \hat{l}_y&=-\mathrm{i}\cos\phi\frac{\partial}{\partial\theta}+\mathrm{i}\sin\phi\,\mathrm{ctg}\,\theta\frac{\partial}{\partial\phi}\end{aligned}$$

откуда

$$\hat{l}_{\pm} = e^{\pm \mathrm{i}\phi}\left(\pm\frac{\partial}{\partial\theta} + \mathrm{i}\,\mathrm{ctg}\,\theta\frac{\partial}{\partial\phi}\right)$$

Как видим, компоненты орбитального момента зависят только от углов.

Для справок приведем также вид оператора квадрата орбитального момента в угловых переменных

$$\hat{\boldsymbol{l}}^2 = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

Собственные функции

$$\hat{\boldsymbol{l}}^2 Y_{l,m}(\theta,\phi) = l(l+1)Y_{l,m}(\theta\phi)$$
$$\hat{l}_z Y_{l,m}(\theta,\phi) = mY_{l,m}(\theta,\phi)$$

нормированные на единицу,

$$\int\limits_{-1}^{1} d\cos\theta \int\limits_{0}^{2\pi} d\phi Y^*_{l,m}(\theta,\phi)Y_{l,m}(\theta,\phi) = 1$$

называются сферическими гармониками.

В угловых переменных уравнение на собственные значения для проекции момента на ось z

$$\hat{l}_z Y_{l,m}(\theta,\phi) = -\mathrm{i}\frac{\partial}{\partial\phi}Y_{l,m}(\theta,\phi) = mY_{l,m}(\theta,\phi)$$

Легко интегрируется при разделении переменных, так что

$$Y_{l,m}(\theta,\phi) = e^{\mathrm{i}m\phi}Y_{l,m}(\theta)$$

Функции $Y_{l,m}(\theta)$ проше всего найти, используя повышающий оператор, который зануляет старший вектор:

$$\hat{l}_+ Y_{l,l}(\theta,\phi) = 0$$

откуда

$$\frac{\partial}{\partial\theta}Y_{l,l}(\theta) - l\,\mathrm{ctg}\,\theta Y_{l,l}(\theta) = 0$$

с решением

$$Y_{l,l}(\theta,\phi) = C_l \sin^l\theta e^{\mathrm{i}l\phi}$$

гДе нормировоч ную константу C_l определим, взяв интеграл

$$I_l = \int\limits_{-1}^{1} d\cos\theta \int\limits_{0}^{2\pi} d\phi \sin^{2l}(\theta)$$

Проведем и нтегрирование по частям:

$$I_l = 2\pi\int\limits_{-1}^{1}\sin^{2l}\theta d\cos\theta = -2\pi 2l\int\limits_{\pi}^{0}\cos\theta\sin^{2l-1}\theta\cos\theta d\theta = 2l\left[\tilde{I}_{l-1} - \tilde{I}_l\right]$$

где после переворота пределов интегрирован ия мы ввели

$$\tilde{I}_l = 2\pi\int\limits_{0}^{\pi}\sin^{2l+1}\theta d\theta$$

Для этого интеграла аналогично находим

$$\tilde{I}_l = -2\pi \int_0^\pi \sin^{2l}\theta d\cos\theta = 2l \int_0^\pi \cos^2\theta \sin^{2l-1} d\theta = 2l\left[\tilde{I}_{l-1} - \tilde{I}_l\right]$$

Получаем рекуррентное соотношение

$$\tilde{I}_l = \frac{2l}{2l+1}\tilde{I}_{l-1} = \frac{2^2 l^2}{(2l)(2l+1)}\tilde{I}_{l-1}, \quad l \in \mathbb{N}$$

причем

$$\tilde{I}_0 = 4\pi$$

и следовательно,

$$\tilde{I}_l = \frac{2^{2l}(l!)^2}{(2l+1)!}4\pi$$

Отсюда

$$I_l = 2l\left[\frac{2l+1}{2l}\tilde{I}_l - \tilde{I}_l\right] = \tilde{I}_l$$

сферические функции

(Перенесу в дополнения потом!!! сюда пару строк добавлю и все)

Сферическая функция для старшего вектора -

$$Y_{l,l}(\theta,\phi) = (-1)^l \sqrt{\frac{(2l+1)!}{4\pi}}\frac{1}{2^l l!}\sin^l\theta e^{\mathrm{i}l\phi}$$

где фактор $(-1)^l$ определяет общепринятое соглашение о фазе. Она нормирована на единицу.

Сферические гармоники с меньшими значениями проекции момента получаются действием понижающего оператора.

$$\hat{l}_-|l,l\rangle = \sqrt{l(l+1)-l(l-1)}|l,l-1\rangle = \sqrt{2l}|l,l-1\rangle$$
$$\hat{l}_-|l,l-1\rangle = \sqrt{l(l+1)-(l-1)(l-2)}|l,l-2\rangle = \sqrt{2(2l-1)}|l,l-2\rangle$$

так что

$$\hat{l}_-^2|l,l\rangle = \sqrt{2l(2l-1)2}|l,l-2\rangle$$
$$\hat{l}_-|l,l-2\rangle = \sqrt{l(l+1)-(l-2)(l-3)}|l,l-3\rangle = \sqrt{3(2l-2)}|l,l-3\rangle$$

или

$$\hat{l}_-^3|l,l\rangle = \sqrt{2l(2l-1)(2l-2)2\cdot 3}|l,l-3\rangle$$

по индукции

$$|l,l-m\rangle = \sqrt{\frac{(2l-m)!}{(2l)!m!}}\hat{l}_-^m|l,l\rangle$$

В частности,

$$Y_{l,0}(\theta,\phi) = \frac{1}{\sqrt{(2l)!}}\hat{l}_-^l Y_{l,l}(\theta,\phi)$$

В явном виде

$$\hat{l}_- Y_{l,m}(\theta,\phi) = e^{-\mathrm{i}\phi}\left(-\frac{\partial}{\partial\theta} + \mathrm{i}\,\mathrm{ctg}\,\theta\frac{\partial}{\partial\phi}\right)e^{\mathrm{i}m\phi}Y_{l,m}(\theta) =$$

$$e^{\mathrm{i}(m-1)\phi}\left(-\frac{\partial}{\partial\theta}-m\operatorname{ctg}\theta\right)Y_{l,m}(\theta)=e^{\mathrm{i}(m-1)\phi}\left(\frac{1}{(\sin\theta)^{m-1}}\frac{\partial}{\partial\cos\theta}\sin^m\theta\right)Y_{l,m}(\theta)$$

Отсюда получаем

$$\hat{l}_-^l Y_{l,l}(\theta,\phi)=\frac{\partial^l}{\partial\cos\theta^l}\sin^l\theta Y_{l,l}(\theta)=C_l\frac{\partial^l}{\partial\cos\theta^l}\sin^{2l}\theta$$

Собирая множители,

$$Y_{l,0}(\theta,\phi)=\sqrt{\frac{2l+1}{4\pi}}\frac{(-1)^l}{2^l l!}\frac{d^l}{d\cos\theta^l}\sin^{2l}\theta$$

Согласно стандартному определению полижомами Лежсаждра называют функци и

$$P_l(\xi)\stackrel{\text{def}}{=}\frac{(-1)^l}{2^l l!}\frac{d^l}{d\xi^l}\left(1-\xi^2\right)^l$$

Н

$$Y_{l,0}(\theta,\phi)=\sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta)$$

Так как сферические гармоники, являющиеся собственным и векторами, ортогональны и нормированы на единицу, для полиномов Лежандра автоматически находим

$$\int\limits_{-1}^{1}d\xi P_l(\xi)P_{l'}(\xi)=\frac{2}{2l+1}\delta_{ll'}$$

Кроме того отмети м следующее свойство этих полиномов

$$P_l(1)=1$$

Что следует из того, что ненулевой вклад при $\xi=1$ дает лишь слагаемое с н улевой степен ью фактора $(1-\xi^2)$, и поэтому нужно многократно дифференцировать лишь степень этого фактора, что и при водит к сокращению численного множителя в (8.21)

Состояния $Y_{l,m}(\theta,\phi)$ с $m>0$ обычно находят с помощью действия повышающего опе-

$$\begin{aligned}\hat{l}_+Y_{l,m}(\theta,\phi)=&e^{\mathrm{i}\phi}\left(\frac{\partial}{\partial\theta}+\mathrm{i}\operatorname{ctg}\theta\frac{\partial}{\partial\phi}\right)e^{\mathrm{i}m\phi}Y_{l,m}(\theta)=\\&=-e^{\mathrm{i}(m+1)\phi}\left\{(\sin\theta)^{m+1}\frac{\partial}{\partial\cos\theta}\frac{1}{\sin^m\theta}\right\}Y_{l,m}(\theta)=\\&=\sqrt{l(l+1)-m(m+1)}Y_{l,m}(\theta,\phi)\\\hat{l}_+^mY_{l,0}(\theta)=&e^{\mathrm{i}m\phi}(-1)^m\sqrt{\frac{2l+1}{4\pi}}\sin^m\theta\frac{d}{d\cos\theta^m}P_l(\theta)\end{aligned}$$

а с другой

(???)

В итоге,

$$Y_{l,m}(\theta,\phi)=e^{\mathrm{i}m\phi}(-1)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_{l,m}(\cos\theta),\quad 0\leqslant m\leqslant l$$

Основы квантового момента импульса по общей физике

(добавлю киселева или Ландау, тут важная теория все-таки)

В то же время другая физическая величина — момент импульса L — для любой системы может принимать только определенный, дискретный ряд значений.

Момент импульса характеризует вращательное (угловое) движение.

При изучении такого движения удобно пользоваться полярной системой координат (рис. 6.1).

в этой системе положение точки характеризуется расстоянием r от начала отсчета, полярным углом θ между полярной осью z и радиусом-вектором $\mathbf{r}$ и азимутальным углом φ, отсчитываемым в плоскости xy от оси x.

волновая функция ψ_{lz}, описываюшая состояние с определенным значен ием проекции l_z на ось z аналогична плоской волне де бройля $\exp\left[i\left(p_x/\hbar\right)z\right]$: роль координаты играет азимутальный угол φ (угол поворо

(????)

случае, если $L_z/\hbar$ принимает целочисленные значения.

Следовательно, L_z, в отличие от проекции импульса p_z, может принимать только дискретные значения:

$$L_z = m_l\hbar, \qquad \text{где} \qquad m_l = 0, \pm1, \pm2, ...$$

Таким образом, проекция момента импульса на любую ось Квантуется и равна целому числу постоянных Планка (на рис. 6.2 дано схематическое изображение квантования проекции l_z момента импульса $\mathbf{l}$ на ось z).

квантование проекции момента означает, что вектор квантового момента импульса не может иметь произвольного направления по отношению к любому фиксированному направлению в пространстве.

этот факт получил название пространственного квантования.

оно выглядит крайне необычно: поскольку направление оси z можно выбрать пройзвольно, то проекции момента на два различных направления (z и z') квантуются одинаково.

возможные значения проекции момента на оси x и y также определяются формулой (6.3).

Может показаться, что квантование проекции L_z приводит к тому, что вектор L составляет лишь определенные углы с осью, как это схематично показано на рис. 6.2.

Однако полученный результат имеет совсем другой смысл.

Формула (6.3) показывает, что при измерении проекции момента импульса мы в результате опыта обязательно получим число, являющееся кратным $\hbar$.

Однако значение L_z до этого вовсе не должно быть равно целому числу $\hbar$.

До и после опыта ψ -функции вовсе не обязаны совпадать.

Мы вправе лишь утверждать, что ψ -функция состояния, имевшегося до опыта, т. е. ψ -функция любого физического состояния, может быть представлена в виде суперпозиции собственных решений:

$$\psi = \sum_m c_m\psi_m = \sum_m c_m\frac{1}{\sqrt{2\pi}}e^{im\varphi}$$

где множитель $1/\sqrt{2\pi}$ возникает как результат нормировки фунКций ψ_m.

Система, описываемая такой ψ -функцией, не обладает определенной проекцией момента L.

Вектор $\mathbf{L}$ может быть направлен произвольным образом, но при измерении L_z всегда будет найдено какое-то одно из m значений, входящих в сумму (6.4).

Вероятность найти значение $L_z = m\hbar$ определяется, как всегда, величиной $|c_m|^2$.

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ва сталкиваемся с действием квантовомеханического принципа неопределенностей.

Проекция момента не может быть больше его абсолютного значения.

Поэтому при фиксированной величине модуля момента возможные значения числа m_l ограничены сверху числом l. Если l задано, то проекция момента может принимать $2l+1$ значений. Найдем возможные значения момента импульса. Средние значения проекций L_x, L_y и L_z, как и любых других величин, могут иметь в данном состоянии определенные значения.

Если никаких предварительных операций для фиксации проекции момента на

какое-либо направление не производилось (нет выделенной поляризации частиц), то все направления равноправны и средние значения квадратов проекций момента импульса одинаковы:

$$\left\langle L_x^2 \right\rangle = \left\langle L_y^2 \right\rangle = \left\langle L_z^2 \right\rangle$$

Это утверждение вместе с правилом квантования проекции момента (6.3) позволяет определить возможные значения квадрата момента импульса.

Среднее значение квадрата момента, как и в классической механике, равно сумме средних значений квадратов проекций.

Учитывая равенство (6.5), получим

$$\left\langle \mathbf{L}^2 \right\rangle = \left\langle L_x^2 \right\rangle + \left\langle L_y^2 \right\rangle + \left\langle L_z^2 \right\rangle = 3 \left\langle L_z^2 \right\rangle$$

При любой ориентации момента его квадрат имеет одну и ту же величину.

Следовательно,

$$L^2 = \left\langle \mathbf{L}^2 \right\rangle = 3 \left\langle L_z^2 \right\rangle$$

Все значения L_z равновероятны, если никакого отбора по возможным состояниям не производилось.

Поэтому среднее значение $\langle L_z^2 \rangle$ равно сумме всех $2l+1$ возможных значений $\langle L_z^2 \rangle$ от $l\hbar$ до - $\hbar$, деленной на их полное число:

$$\left\langle L_z^2 \right\rangle = \hbar^2 \frac{l^2 + (l-1)^2 + \cdots + (-l)^2}{2l+1} = \frac{2\hbar^2}{2l+1} \left(1^2 + 2^2 + 3^2 + \cdots + l^2\right) =$$
$$= \frac{2\hbar^2}{2l+1} \frac{l(l+1)(2l+1)}{6} = \frac{\hbar^2}{3} l(l+1)$$

Здесь мы использовали известное выражение для суммы квадратов целых чисел от 1 до l.

Подставив полученное значение $\langle L_z^2 \rangle$ в (6.6), найдем

$$L^2 = \hbar^2 l(l+1)$$

Равенство (6.8) определяет закон квантования квадрата момента импульса, т. е. его длину.

Число m_l, от которого зависят значения проекции момента, называется магнитным квантовым числом.

Этот термин обусловлен тем, что, как мы увидим в дальнейшем, проекция магнитного момента, создаваемого движением заряженной частицы, пропорциональна проекции момента импульса этой частицы, определяемого числом m_l.

Максимальное значение магнитного квантового числа $m_{\max} = l$, а минимальное $m_{\min} = -l$.

Число l определяющее возможные значения квадрата момента, называется орбитальным квантовым числом.

Отметим еще одно отличие квантового момента от классического.

Максимальное значение проекции квантового момента $\hbar l$ не равно модулю момента $\hbar\sqrt{l(l+1)}$, а меньше его.

Мы уже подчеркивали, что в силу соотношения неопределенностей у микрочастицы не могут быть одновременно известны проекции момента на две различные оси.

Зафиксировав состояние с определенным L_z, мы вносим неопределенность в проекции L_x и L_y.

В квантовой механике задание L^2 и одной из проекций момента импульса полностью определяет вращательное состояние тела.

Как догадаться про это?

4.5.2 Transformation of States Under Rotations

Суть (!?!?!?!?)

(очень важно, в 1ю напишу!!!)

7.2.1. Преобразование состояний.

Как мы знаем, в классическом пределе малых флуктуаций волновая функция состояния, амплитуда вероятности, переходит в волну материи, фаза которой пропорциональна классическому действию для корпускул, которые движутся по лучам согласно законам геометрической оптики. Однако пример поля - электромагнитные волны показывает, что амплитуда волны обладает еще и такой характеристикой, как поляризация. Действительно, электрическое и магнитное поля являются векторами. Следовательно, амплитуда вероятности при квантовании будет характеризоваться не только своими модулем и фазой, зависящими от координат и импульсов, но и поляризацией. Поэтому частицы, составляющие, например, электромагнитное поле в квантовой механике, кроме координаты и импульса имеют еще и наблюдаемую величину λ, которая в классике соответствует поляризации волн. Для частиц с поляризацией базисом состояний может служить набор векторов с определенными значениями координаты частицы и ее поляризации $|\boldsymbol{r}, \lambda\rangle$ Тогда состоянию $|\Psi\rangle$ соответствует волновая функция

$$\langle \boldsymbol{r}, \lambda | \Psi \rangle = \Psi_\lambda(\boldsymbol{r}).$$

Особенностью преобразования квантовых состояний при вращениях является определение закона преобразования поляризаций частиц.

Скалярные частицы.

Скалярными называются частицы, у которых нет поляризации, так что имеет место стандартное определение преобразований состояния при вращениях:

$$\left\langle \boldsymbol{r}^{\phi}|\Psi^{\phi}\right\rangle = \langle \boldsymbol{r}|\Psi\rangle, \quad \Psi^{\phi}\left(\boldsymbol{r}^{\phi}\right) = \Psi(\boldsymbol{r}),$$

где

$$\hat{R}|\Psi\rangle = \left|\Psi^{\phi}\right\rangle, \quad \hat{R}|\boldsymbol{r}\rangle = \left|\boldsymbol{r}^{\boldsymbol{\phi}}\right\rangle = \left|\mathcal{R}^{\mathrm{T}}\boldsymbol{r}\right\rangle$$

где $\mathcal{R}$ - матрица поворотов в классике. Отсюда можно также записать

$$\Psi^{\phi}(\boldsymbol{r}) = \Psi(\mathcal{R}\boldsymbol{r}),$$

поскольку

$$\Psi^{\phi}(\boldsymbol{r}) = \langle \boldsymbol{r}|(\hat{R}|\Psi\rangle) = \left(\hat{R}^{\dagger}|\boldsymbol{r}\rangle\right)^{\dagger}|\Psi\rangle = (|\mathcal{R}\boldsymbol{r}\rangle)^{\dagger}|\Psi\rangle = \mathrm{e}^{\frac{i}{\hbar}\hat{\boldsymbol{L}}\cdot\boldsymbol{\phi}}\Psi(\boldsymbol{r})$$

есть не что иное, как координатное представление оператора вращений, где

$$\hat{\boldsymbol{L}} = -\mathrm{i}\hbar(\boldsymbol{r}\times\boldsymbol{\nabla})$$

В итоге

$$\Psi^{\phi}(\boldsymbol{r}) = \mathrm{e}^{\frac{i}{\hbar}\hat{\boldsymbol{L}}\cdot\boldsymbol{\phi}}\Psi(\boldsymbol{r}) = \Psi(\mathcal{R}\boldsymbol{r}).$$

В справедливости этого тождества можно убедиться прямыми вычислениями. Например, при $\phi \to 0$ инфинитезимально находим

$$\{1 + \boldsymbol{\phi}\cdot(\boldsymbol{r}\times\boldsymbol{\nabla})\}\Psi(\boldsymbol{r}) = \Psi(\boldsymbol{r} - \boldsymbol{r}\times\boldsymbol{\phi}),$$

и, переставляя порядок вычисления смешанного произведения слева, получаем верное тождество

$$\Psi(\boldsymbol{r}) - (\boldsymbol{r}\times\boldsymbol{\phi})\cdot\boldsymbol{\nabla}\Psi(\boldsymbol{r}) = \Psi(\boldsymbol{r} - \boldsymbol{r}\times\boldsymbol{\phi}).$$

Векторные частицы.

Векторными называются частицы, состояние которых характеризуются и координатой и единичным вектором поляризации ϵ. Независимых поляризаций может быть несколько, так что их можно нумеровать маркером λ, и поэтому волновая функция векторной частицыВектор:

$$\langle \boldsymbol{r}, \epsilon_{\lambda}|\Psi\rangle = \boldsymbol{\Psi}_{\lambda}(\boldsymbol{r}) \quad \text{или} \quad \langle \boldsymbol{r}, \boldsymbol{\epsilon}|\Psi\rangle = \boldsymbol{\epsilon}\cdot\boldsymbol{\Psi}(\boldsymbol{r}).$$

Вектор поляризации при вращениях преобразуется так же, как координата, так что

$$\hat{R}|\boldsymbol{r}, \boldsymbol{\epsilon}\rangle = \left|\boldsymbol{r}^{\boldsymbol{\phi}}, \boldsymbol{\epsilon}^{\boldsymbol{\phi}}\right\rangle = \left|\mathcal{R}^{\mathrm{T}}\boldsymbol{r}, \mathcal{R}^{\mathrm{T}}\boldsymbol{\epsilon}\right\rangle.$$

В силу унитарности оператора вращений

$$\hat{R}\hat{R}^{\dagger} = \mathbb{1}$$

по-прежнему имеет место тождество

$$\left\langle \boldsymbol{r}^{\boldsymbol{\phi}}, \boldsymbol{\epsilon}^{\boldsymbol{\phi}}|\Psi^{\boldsymbol{\phi}}\right\rangle = \langle \boldsymbol{r}, \boldsymbol{\epsilon}|\Psi\rangle.$$

Отсюда

$$\left(\mathcal{R}^{\mathrm{T}}\boldsymbol{\epsilon}\right)\cdot\boldsymbol{\Psi}^{\boldsymbol{\phi}}\left(\mathcal{R}^{\mathrm{T}}\boldsymbol{r}\right) = \boldsymbol{\epsilon}\cdot\boldsymbol{\Psi}(\boldsymbol{r})$$

или после использования равенства

$$\left(\mathcal{R}^{\mathrm{T}}\epsilon\cdot\Psi^{\phi}\right)=\mathcal{R}^{\mathrm{T}}_{\lambda\rho}\epsilon_{\rho}\Psi^{\phi}_{\lambda}=\epsilon_{\rho}\mathcal{R}_{\rho\lambda}\Psi^{\phi}_{\lambda}=\epsilon\cdot\left(\mathcal{R}\Psi^{\phi}\right)$$

и подходящей замены переменных $r\to\mathcal{R}r$ получаем

$$\mathcal{R}\Psi^{\phi}(r)=\Psi(\mathcal{R}r)\Leftrightarrow\Psi^{\phi}(r)=\mathcal{R}^{\mathrm{T}}\Psi(\mathcal{R}r),$$

или в тензорной записи

$$\boldsymbol{\Psi}^{\phi}_{\lambda}(\boldsymbol{r})=\mathcal{R}^{\mathrm{T}}_{\lambda\mu}\boldsymbol{\Psi}_{\rho}(\mathcal{R}\boldsymbol{r}),$$

где согласно (7.27) преобразование аргумента функции сводится к действию оператора орбитальных вращений,

$$\Psi_{\rho}(\mathcal{R}r)=\mathrm{e}^{\frac{i}{\hbar}\hat{L}\cdot\phi}\Psi_{\rho}(\boldsymbol{r}),$$

и

$$\Psi^{\phi}_{\lambda}(r)=\mathcal{R}^{\mathrm{T}}_{\lambda\rho}\mathrm{e}^{\dot{j}\hat{L}\cdot\phi}\Psi_{\rho}(\boldsymbol{r}),$$

Матрица поворотов нам известна, так как она определяется поворотами координат. Для бесконечно малых преобразований в (7.33) положим, что

$$\mathcal{R}^{\mathrm{T}}=\mathbb{1}+\mathrm{i}(\boldsymbol{\phi}\cdot\hat{\boldsymbol{s}}),$$

где векторная (3×3)-матрица $\hat{\boldsymbol{s}}$ определяется из равенства линейных по углу правых и левых частей равенства

$$\mathcal{R}^{\mathrm{T}}_{\alpha\beta}=\delta_{\alpha\beta}+\epsilon_{\alpha\beta\gamma}\phi^{\gamma}=\delta_{\alpha\beta}+\mathrm{i}\left(s_{\gamma}\right)_{\alpha\beta}\phi^{\gamma}.$$

Поэтому

$$\left(\hat{s}_{\gamma}\right)_{\alpha\beta}=-\mathrm{i}\epsilon_{\alpha\beta\gamma}.$$

Эта матрица эрмитова:

$$\left(\hat{\boldsymbol{s}}^{\dagger}_{\gamma}\right)_{\alpha\beta}=\left(\hat{\boldsymbol{s}}^{*}_{\gamma}\right)_{\beta\alpha}=\left(\hat{\boldsymbol{s}}_{\gamma}\right)_{\alpha\beta},$$

здесь мы использовали антисимметрию тензора Леви-Чивиты. Покажем, что для этой матрицы имеют место соотношения коммутации

$$[\hat{\boldsymbol{s}}_{\alpha},\hat{\boldsymbol{s}}_{\beta}]=\mathrm{i}\epsilon_{\alpha\beta\gamma}\hat{\boldsymbol{s}}_{\gamma}.$$

В самом деле, слева в этой формуле стоит матричное выражение с индексами

$$\begin{aligned}&\{\mu,\lambda\}\\&(-\mathrm{i})^2\left(\epsilon_{\alpha\mu\nu}\epsilon_{\beta\nu\lambda}-\epsilon_{\beta\mu\nu}\epsilon_{\alpha\nu\lambda}\ \right)=\\&\quad=\delta_{\alpha\beta}\delta_{\mu\lambda}-\delta_{\alpha\lambda}\delta_{\mu\beta}-\delta_{\alpha\beta}\delta_{\mu\lambda}+\delta_{\alpha\mu}\delta_{\beta\lambda}=\delta_{\alpha\mu}\delta_{\beta\lambda}-\delta_{\alpha\lambda}\delta_{\mu\beta}.\end{aligned}$$

Справа же имеем

$$\mathrm{i}(-\mathrm{i})\epsilon_{\alpha\beta\gamma}\epsilon_{\gamma\mu\lambda}=\delta_{\alpha\mu}\delta_{\beta\lambda}-\delta_{\alpha\lambda}\delta_{\mu\beta},$$

и тождество доказано. В матричных обозначениях для конечных вращений находим

$$\mathcal{R}^{\mathrm{T}}(\phi)=\mathrm{e}^{\mathrm{i}\hat{\boldsymbol{\beta}}\cdot\boldsymbol{\phi}}.$$

В итоге, преобразование волновой функции частицы с вектором поляризации (7.31) эквивалентно

$$\Psi^{\phi}(r)=\mathrm{e}^{\frac{i}{\hbar}(\hat{L}+\hat{S})\cdot\phi}\Psi(r),$$

где матричный оператор размерности действия

$$\hat{\boldsymbol{S}} = \hbar \hat{\boldsymbol{s}}$$

называется спином векторной частицы, а сумма

$$\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}$$

- полным моментом импульса частицы. В принятых обозначениях преобразованная при вращениях волновая функция выражается через исходную волновую функцию действием оператора вращений с генератором полного момента количества движения

$$\Psi^{\phi}(r) = \mathrm{e}^{\frac{1}{\hbar}\cdot\hat{J}\cdot\phi}\Psi(r),$$

так что физический смысл оператора спина, возникающего из-за введения поляризации волновой функции, есть собственный момент количества движения частицы.

Так как в координатном представлении дифференциальный оператор орбитального момента коммутирует с постоянной матрицей спина

$$\left[\hat{\boldsymbol{L}}_{\alpha}, \hat{\boldsymbol{S}}_{\beta}\right] = 0,$$

а коммутационные соотношения для спиновой матрицы идентичны соотношениям для орбитального момента, для полного момента импульса [1] получаем

$$\left[\hat{\boldsymbol{J}}_{\alpha}, \hat{\boldsymbol{J}}_{\beta}\right] = \mathrm{i}\hbar\epsilon_{\alpha\beta\gamma}\hat{\boldsymbol{J}}_{\gamma},$$

которые совпадают с коммутационными соотношениями как орбитального момента, так и спина.

Зададимся вопросом: является ли случай векторной частицы единственным примером, когда у частицы может быть поляризация? Кроме вектора, который представляет собой тензор первого ранга, существуют и тензоры второго ранга и тензоры высших рангов. Но тогда как описываются преобразования волновых функций таких полей при поворотах в евклидовом пространстве? И каков допустимый спектр поляризаций частиц?

Операторное квантование момента количества движения согласно коммутационным соотношениям (7.42) позволит нам определить допустимые значения момента количества движения, т.е. найти базис волновых функций в отношении их преобразований при поворотах и построить схему описания квантовых состояний с различными значениями спина и орбитального момента.

Преобразование операторов.

Согласно общей схеме при каноническом квантовании оператор вращений в квантовой механике имеет генератор так что

$$\hat{\boldsymbol{\Gamma}} = \frac{1}{\hbar}\hat{\boldsymbol{L}},$$

$$\hat{R} = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{L}\cdot\phi}.$$

Для операторов, построенных из координат и импульсов, преобразование имеет вид

$$\hat{F}_{\phi} = \hat{R}\hat{F}\hat{R}^{\dagger} = \mathcal{R}(\hat{F}).$$

Рассмотрим два важнейших случая. 1. Скалярная наблюдаемая C. В классической механике скалярные величины не преобразуются при вращениях. Поэтому

$$\mathcal{R}(C) = C.$$

Значит, и в квантовой механике скалярная наблюдаемая не преобразуется при действии оператора вращений

$$\hat{C}_\phi = \hat{C}.$$

Подставляя в (7.44) инфинитезимальный оператор вращений

$$\hat{R} = \mathbb{1} + \frac{\mathrm{i}}{\hbar}\hat{\boldsymbol{L}} \cdot \phi, \quad \phi \to 0,$$

находим коммутатор оператора орбитального момента с произвольной скалярной наблюдаемой

$$[\hat{\boldsymbol{L}}, \hat{\boldsymbol{C}}] = 0.$$

2. Векторная наблюдаемая $\boldsymbol{A}$. В классической механике векторные величины преобразуются так же, как и координаты:

$$A^\phi_\alpha = \mathcal{R}_{\alpha\beta} A_\beta,$$

так что квантовый векторный оператор преобразуется при вращениях как

$$\hat{\boldsymbol{A}}^\phi_\alpha = \hat{R}\hat{\boldsymbol{A}}_\alpha \hat{R}^\dagger = \mathcal{R}_{\alpha\beta}\hat{\boldsymbol{A}}_\beta.$$

Для бесконечно малых поворотов в правой стороне (7.49) получаем

$$\mathcal{R}_{\alpha\beta}\hat{\boldsymbol{A}}_\beta \approx \hat{\boldsymbol{A}}_\alpha - \epsilon_{\alpha\beta\gamma}\hat{\boldsymbol{A}}_\beta \boldsymbol{\phi}_\gamma, \quad \phi \to 0,$$

в то время как

$$\hat{R}\hat{\boldsymbol{A}}_\alpha \hat{R}^\dagger \approx \hat{\boldsymbol{A}}_\alpha + \frac{\mathrm{i}}{\hbar}\left[\hat{\boldsymbol{L}}_\gamma \boldsymbol{\phi}_\gamma, \hat{\boldsymbol{A}}_\alpha\right].$$

Сравнивая два предыдущих выражения, находим

$$\left[\hat{\boldsymbol{L}}_\gamma, \hat{\boldsymbol{A}}_\alpha\right] = \mathrm{i}\hbar\epsilon_{\alpha\beta\gamma}\hat{\boldsymbol{A}}_\beta,$$

так что после переобозначения индексов суммирования получаем общее выражение для коммутатора мамента цмпульса с векторной наблюдаемой:

$$\left[\hat{\boldsymbol{L}}_\alpha, \hat{\boldsymbol{A}}_\beta\right] = \mathrm{i}\hbar\epsilon_{\alpha\beta\gamma}\hat{\boldsymbol{A}}_\gamma.$$

Обычно определяют безразмерный векторный оператор

$$\hat{\boldsymbol{l}} = \frac{1}{\hbar}\hat{\boldsymbol{L}},$$

так что, в частности, из (7.50) следуют коммутационные соотношения для оператора момента импульса

$$\left[\hat{\boldsymbol{l}}_\alpha, \hat{\boldsymbol{l}}_\beta\right] = \mathrm{i}\epsilon_{\alpha\beta\gamma}\hat{\boldsymbol{l}}_\gamma.$$

Последнее равенство можно также установить посредством выкладок в явном виде, пользуясь выражением для оператора

$$\hat{\boldsymbol{L}}_\alpha = \epsilon_{\alpha\beta\gamma}\hat{\boldsymbol{r}}_\beta\hat{\boldsymbol{p}}_\gamma.$$

Важным приложением общих результатов являются коммутационные соотношения генераторов поворотов с квадратом момента импульса

$$\left[\hat{\boldsymbol{l}}_\alpha, \hat{\boldsymbol{l}}^2\right] = 0,$$

как и должно быть для скалярного оператора $\hat{l}^2$.

Как догадаться про это?

4.5.3 Concept of Spin

Суть (!?)

(в 1ю продублирую.)

Спин по Киселеву

Рассмотрим собственный момент импульса частицы, спин, $s = \frac{1}{2}$. В этом случае соответствующая спиновая матрица представляется в виде

$$\hat{\boldsymbol{s}} = \frac{1}{2}\hat{\boldsymbol{\sigma}},$$

где $\boldsymbol{\sigma}$ - матрицы Паули [1]. Найдем явный вид матриц Паули, используя общие выражения для матричных элементов момента импульса (8.9), (8.11). Базис спиновых состояний для краткости обозначений записывают как

$$\left|\frac{1}{2}, +\frac{1}{2}\right\rangle = |+\rangle, \quad \left|\frac{1}{2}, -\frac{1}{2}\right\rangle = |-\rangle,$$

причем это-собственные векторы проекции спина

$$\hat{s}_z|+\rangle = \frac{1}{2}|+\rangle, \quad \hat{s}_z|-\rangle = -\frac{1}{2}|-\rangle.$$

Следовательно, эта матрица в рассматриваемом базисе имеет диагональный вид

$$\hat{\boldsymbol{s}}_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Согласно (8.11) ненулевые матричные элементы повышающего и понижающего операторов

$$\langle + |\hat{s}_+| - \rangle = \sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right) - (-1)\frac{1}{2}\left(-\frac{1}{2}+1\right)} = 1,$$

$$\langle - |\hat{s}_-| + \rangle = (\langle + |\hat{s}_+| - \rangle)^\dagger = 1,$$

откуда

$$\hat{\boldsymbol{s}}_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{\boldsymbol{s}}_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

Тогда

$$\hat{\boldsymbol{s}}_x = \frac{1}{2}\left(\hat{\boldsymbol{s}}_+ + \hat{\boldsymbol{s}}_-\right) = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

и

$$\hat{\boldsymbol{s}}_y = \frac{1}{2\mathrm{i}}\left(\hat{\boldsymbol{s}}_+ - \hat{\boldsymbol{s}}_-\right) = \frac{1}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}.$$

Поэтому сигма-матрицы Паули - это

$$\hat{\boldsymbol{\sigma}}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\boldsymbol{\sigma}}_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \hat{\boldsymbol{\sigma}}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Поскольку частица со спином $\frac{1}{2}$, которую называют спинором, обладает двумя поляризациями [1]

$$|\mathfrak{e}_1\rangle = |+\rangle, \quad |\mathfrak{e}_2\rangle = |-\rangle, \quad |\mathfrak{e}_\alpha\rangle, \quad \alpha = \{1, 2\},$$

можно определить состояие поляризаций как

$$\langle\theta| = \langle\mathfrak{e}_\alpha|\,\theta^\alpha,$$

так что волновая функция нерелятивистского спинора [2]

$$\langle \boldsymbol{r}, \mathfrak{e}_\alpha|\Psi\rangle = \psi_\alpha(\boldsymbol{r})$$

- это так называемый двухкомпонентный спинор Паули, которой преобразуется как контрвариантный вектор двумерного пространства спиноров, и его по договоренности обычно трактуют в матричной записи как столбец. При поворотах спинор преобразуется согласно

$$\psi^\phi_\alpha(\boldsymbol{r}) = \left\{\mathrm{e}^{\mathrm{i}\hat{\mathbf{s}}\cdot\boldsymbol{\phi}}\right\}^{\cdot\beta}_{\alpha}\psi_\beta\left(\boldsymbol{r}^\phi\right),$$

где мы указали матричные индексы в явном виде, и, при этом, указали порядок следования индексов в матричном умножении с помощью символа - Так как по построению

$$\langle \boldsymbol{r}, \theta|\Psi\rangle = \theta^\alpha\psi_\alpha(\boldsymbol{r})$$

- инвариант при вращениях, спинор поляризации θ^α (строка) преобразуется как

$$\theta^\beta = \theta^\alpha_\phi\left\{\mathrm{e}^{\mathrm{i}\hat{\mathbf{s}}\cdot\boldsymbol{\phi}}\right\}^{\bullet\beta}_{\alpha} \Leftrightarrow \theta^\beta_\phi = \theta^\alpha\left\{\mathrm{e}^{-\mathrm{i}\hat{\mathbf{s}}\cdot\boldsymbol{\phi}}\right\}^{\bullet\beta}_{\alpha}.$$

В матричных обозначениях

$$\psi^\phi(\boldsymbol{r}) = \hat{R}_S\cdot\psi(\mathcal{R}\boldsymbol{r}), \quad \theta_{\boldsymbol{\phi}} = \theta\cdot\hat{R}^\dagger_S, \quad \hat{R}_S = \mathrm{e}^{\mathrm{i}\hat{\mathbf{s}}\cdot\boldsymbol{\phi}}$$

причем ψ_α - контрвектор двумерного спинорного пространства, который преобразуется матрицей $\hat{R}_S$, а θ^α - ковектор, который преобразуется обратной матрицей $\hat{R}^{-1}_S = \hat{R}^\dagger_S$.

Для вычисления матричной экспоненты установим два факта:

1) коммутационные соотношения

$$[\hat{\boldsymbol{\sigma}}_a, \hat{\boldsymbol{\sigma}}_b] = 2\mathrm{i}\epsilon_{abc}\hat{\boldsymbol{\sigma}}_c$$

следуют из коммутационных соотношений для момента импульса;

2) антикоммутационные соотношения

$$\{\hat{\sigma}_a, \hat{\sigma}_b\} \stackrel{\mathrm{def}}{=} \hat{\sigma}_a\hat{\sigma}_b + \hat{\sigma}_b\hat{\sigma}_a = 2\delta_{ab}$$

устанавливаются прямыми вычислениями произведений матриц Паули.

Поскольку

$$\hat{\boldsymbol{\sigma}}_a\hat{\boldsymbol{\sigma}}_b = \frac{1}{2}\left[\hat{\boldsymbol{\sigma}}_a, \hat{\boldsymbol{\sigma}}_b\right] + \frac{1}{2}\left\{\hat{\boldsymbol{\sigma}}_a, \hat{\boldsymbol{\sigma}}_b\right\},$$

находим

$$\hat{\boldsymbol{\sigma}}_a\hat{\boldsymbol{\sigma}}_b = \mathrm{i}\epsilon_{abc}\hat{\boldsymbol{\sigma}}_c + \delta_{ab}.$$

Домножая это тождество на векторы $\boldsymbol{a}_a$ и $\boldsymbol{b}_b$, получаем

$$(\boldsymbol{a}\cdot\hat{\boldsymbol{\sigma}})(\boldsymbol{b}\cdot\hat{\boldsymbol{\sigma}}) = \mathrm{i}(\boldsymbol{a}\times\boldsymbol{b})\cdot\hat{\boldsymbol{\sigma}} + \boldsymbol{a}\cdot\boldsymbol{b},$$

где справа стоит векторное произведение векторов. В частности,

$$(\boldsymbol{\phi}\cdot\hat{\boldsymbol{\sigma}})^2 = \boldsymbol{\phi}^2.$$

Тогда в экспоненте оператора вращений

$$\mathrm{e}^{\mathrm{i}\hat{\boldsymbol{s}}\cdot\boldsymbol{\phi}} = \sum_{n=0}^{\infty} \frac{\mathrm{i}^n}{2^n n!} (\phi \cdot \hat{\boldsymbol{\sigma}})^n$$

четные степени разложения пропорциональны единичной матрице, а нечетные-оператору

$$(\phi \cdot \hat{\boldsymbol{\sigma}}) = |\boldsymbol{\phi}|(\boldsymbol{e} \cdot \hat{\boldsymbol{\sigma}}) = (\boldsymbol{\phi} \cdot \boldsymbol{e})(\boldsymbol{e} \cdot \hat{\boldsymbol{\sigma}}),$$

где $\boldsymbol{e}$-единичный вектор вдоль оси поворота. Тогда суммирование четных и нечетных степеней дает

$$\mathrm{e}^{\mathrm{i}\hat{\boldsymbol{s}}\cdot\boldsymbol{\phi}} = \cos\left(\frac{1}{2}(\boldsymbol{\phi}\cdot\boldsymbol{e})\right) + \mathrm{i}(\boldsymbol{e}\cdot\hat{\boldsymbol{\sigma}})\sin\left(\frac{1}{2}(\boldsymbol{\phi}\cdot\boldsymbol{e})\right).$$

При повороте вокруг оси на угол $2\pi = (\boldsymbol{\phi}\cdot\boldsymbol{e})$ получаем $\boldsymbol{r}^{\phi} = r$ и

$$\mathrm{e}^{\mathrm{i}\hat{\boldsymbol{s}}\cdot\phi}\big|_{2\pi} = -1.$$

Значит,

$$\psi_\alpha(\boldsymbol{r})\big|_{2\pi} = -\psi_\alpha(\boldsymbol{r}),$$

т. е. волновая функция спинора меняет знак после поворота на угол 2π. Это свойство, очевидно, является общим для всех частиц с полуцелым спином, которые называются фермионами.

Спиновая метрика (?)

Введем вещественную матрицу $\hat{\epsilon}$,

$$\hat{\epsilon} \overset{\text{def}}{=} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \mathrm{i}\sigma_2, \quad \hat{\epsilon}^2 = -1, \quad \hat{\epsilon}^{-1} = \hat{\epsilon}^{\mathrm{T}} = -\hat{\epsilon},$$

и определим сопряженный к спинору ψ спинор ψ_c с помощью комплексного сопряжения и матричного умножения,

$$\psi_c \overset{\text{def}}{=} -\hat{\epsilon}\psi^* = -\mathrm{i}\sigma_2\psi^*,$$

а затем рассмотрим, как как он преобразуется при поворотах,

$$\psi_c^{\phi} = -\hat{\epsilon}\left(\hat{R}_S\psi\right)^* = \hat{\epsilon}\hat{R}_S^*\hat{\epsilon}^{-1}\left(-\hat{\epsilon}\psi^*\right). = \hat{\epsilon}\hat{R}_S^*\hat{\epsilon}^{-1}\psi_c,$$

Значит, нам необходимо найти матрицу $\hat{\epsilon}\hat{R}_S^*\hat{\epsilon}^{-1}$. При этом, матрица поворотов спиноров $\hat{R}_S$ имеет вид экспоненты (9.13). В общем случае, так как $\hat{\epsilon}\circ\hat{\epsilon}^{-1} = \mathbb{1}$, разложение экспоненты от матрицы в ряд Тейлора приводит к

$$\hat{\epsilon}\circ\exp\{A\}\circ\hat{\epsilon}^{-1} = \hat{\epsilon}\circ\left(\sum_{n=0}^{\infty}\frac{1}{n!}A^n\right)\circ\hat{\epsilon}^{-1} = \sum_{n=0}^{\infty}\frac{1}{n!}\left\{\hat{\epsilon}\circ A\circ\hat{\epsilon}^{-1}\right\}^n = \exp\left\{\hat{\epsilon}\circ A\circ\hat{\epsilon}^{-1}\right\}.$$

В случае матрицы поворотов

$$\hat{R}_S = \exp\left(\frac{\mathrm{i}}{2}\phi(\boldsymbol{\sigma}\cdot\boldsymbol{e})\right),$$

так что

$$\hat{R}_S^* = \exp\left(-\frac{\mathrm{i}}{2}\phi\left(\boldsymbol{\sigma}^*\cdot\boldsymbol{e}\right)\right).$$

Для вычисления $\hat{\epsilon} \circ \boldsymbol{\sigma}^* \circ \hat{\epsilon}^{-1}$ заметим, что матрицы σ_x, σ_z симметричные и вещественные, так что

$$\sigma_x^* = \sigma_x^{\mathrm{T}} = \sigma_x, \quad \sigma_z^* = \sigma_z^{\mathrm{T}} = \sigma_z,$$

а матрица σ_y чисто мнимая и антисимметричная, так что

$$\sigma_y^* = \sigma_y^{\mathrm{T}} = -\sigma_y.$$

Поэтому в силу

$$\sigma_x\hat{\epsilon} = -\hat{\epsilon}\sigma_x, \quad \sigma_z\hat{\epsilon} = -\hat{\epsilon}\sigma_z, \quad \sigma_y\hat{\epsilon} = \hat{\epsilon}\sigma_y,$$

получаем

$$\hat{\epsilon} \circ \boldsymbol{\sigma}^* \circ \hat{\epsilon}^{-1} = \hat{\epsilon} \circ \boldsymbol{\sigma}^{\mathrm{T}} \circ \hat{\epsilon}^{-1} = -\boldsymbol{\sigma}.$$

Значит,

$$\hat{\epsilon}\hat{R}_S^*\hat{\epsilon}^{-1} = \hat{\epsilon}\exp\left(-\frac{\mathrm{i}}{2}\phi\,(\sigma^* \cdot \boldsymbol{e})\right)\hat{\epsilon}^{-1} = \exp\left(-\frac{\mathrm{i}}{2}\phi\left(\hat{\epsilon}\boldsymbol{\sigma}^*\hat{\epsilon}^{-1} \cdot \boldsymbol{e}\right)\right) = \hat{R}_S,$$

и аналогично,

$$\hat{\epsilon}\hat{R}_S^{\mathrm{T}}\hat{\epsilon}^{-1} = \hat{\epsilon}\exp\left(\frac{\mathrm{i}}{2}\phi\left(\boldsymbol{\sigma}^{\mathrm{T}} \cdot \boldsymbol{e}\right)\right)\hat{\epsilon}^{-1} = \exp\left(\frac{\mathrm{i}}{2}\phi\left(\hat{\epsilon}\boldsymbol{\sigma}^{\mathrm{T}}\hat{\epsilon}^{-1} \cdot \boldsymbol{e}\right)\right) = \hat{R}_S^\dagger = \hat{R}_S^{-1}.$$

Напомним, что при использовании матричного умножения контравариантные спиноры ψ_α, которые при матричной записи можно по договоренности считать столбцами $\psi_\alpha\bullet$, преобразуются матрицами $\hat{R}_S$, а ковариантные спиноры ψ^α, которые можно считать строками $\psi^{\bullet\alpha}$, преобразуются обратными матрицами $\hat{R}_S^{-1}$. При этом, R_S - это унитарная матрица:

$$R_S \cdot R_S^\dagger = \mathbb{1}, \quad R_S^\dagger = R_S^{-1},$$

и поэтому эрмитово сопряженный спинор преобразуется как ковариантный. Говорят, что соотношение (9.25) устанавливает эквивалентность транспонированного представления группы поворотов спиноров эрмитово сопряженному представлению этой группы или, в данном случае, еще и эквивалентность транспонированного контравариантного представления ковариантному, а соотношение (9.24) - эквивалентность комплексно сопряженного представления контравариантному спинорному представлению. Итак, при поворотах

$$\psi_c^\phi = \hat{R}_S\psi_c,$$

где мы воспользовались соотношением (9.24). Значит, этот спинор при поворотах преобразуется также, как и сам спинор ψ. Поэтому произведение двух любых спиноров

$$\psi_c^\dagger\chi = \left(-\hat{\epsilon}\psi^*\right)^\dagger\chi = \psi^{\mathrm{T}}(-\hat{\epsilon})^\dagger\chi = \psi^{\mathrm{T}}\hat{\epsilon}\chi = \psi_\alpha\hat{\epsilon}^{\alpha\beta}\chi_\beta$$

является скаляром, т.е. инвариантом группы поворотов спиноров. Значит, формула определяет скалярное произведение двух спиноров. Поэтому согласно общему представлению о метрическом тензоре как о квадратичной инвариантной линейной функции $\hat{\epsilon}^{\alpha\beta}$ - полностью антисимметричный ковариантный тензор второго ранга в двумерном пространстве:

$$\epsilon^{\alpha\beta} = -\epsilon^{\beta\alpha}, \quad \epsilon^{12} = 1.$$

В терминах метрики скалярное произведение двух произвольных спиноров ψ и χ

$$\psi \cdot \chi = \epsilon^{\alpha\beta}\psi_\alpha\chi_\beta.$$

Метрика определяет ковариантные спиноры с верхними индексами

$$\chi^\alpha = \epsilon^{\alpha\beta}\chi_\beta,$$

так что скалярное произведение

$$\psi \cdot \chi = \psi_\alpha \chi^\alpha = -\psi^\beta \chi_\beta.$$

Обратная метрика $\epsilon_{\alpha\beta}$ определяется согласно

$$\epsilon_{\alpha\gamma}\epsilon^{\gamma\beta} = \delta^\beta_\alpha.$$

Очевидно,

$$\epsilon_{\alpha\beta} = -\epsilon_{\beta\alpha}, \quad \epsilon_{12} = -1.$$

Определенный выше спинор ψ_c обозначают также спинором с чертой, который имеет нижний индекс с точкой, так как он преобразуется по представлению, эквивалентному представлению, которое действует в комплексно сопряженном спинорном пространстве:

$$\bar{\psi}^{\dot\alpha} \stackrel{\text{def}}{=} (-\hat\epsilon\psi^*)^{\dot\alpha}$$

Как мы показали, этот спинор при поворотах преобразуется также, как и обычный спинор. Поэтому скаляром будет величина (см. знаки в (9.27))

$$-\chi^\dagger \cdot \psi_c = -\bar\chi^{\dot\alpha}\bar\psi_{\dot\alpha},$$

где мы ввели обозначение для спинора с чертой и с верхним индексом с точкой как эрмитово сопряженного к обычному спинору-столбцу:

$$\bar\chi^{\dot\alpha} = \left(\chi^\dagger\right)^{\dot\alpha}.$$

Элементарно

$$\chi^\dagger = \{\chi^*\}^{\mathrm{T}} = \{\hat\epsilon\,(-\hat\epsilon\chi^*)\}^{\mathrm{T}} = \{\hat\epsilon\bar\chi\}^{\mathrm{T}} = -\bar\chi^{\mathrm{T}}\hat\epsilon.$$

Поэтому

$$-\bar\chi\cdot\bar\psi = \bar\chi^{\mathrm{T}}\hat\epsilon\bar\psi = \bar\chi_{\dot\alpha}\epsilon^{\dot\alpha\dot\beta}\bar\psi_{\dot\beta}, \quad \epsilon^{12} = 1$$

т.е. метрика $\epsilon^{\dot\alpha\dot\beta}$ в спинорных индексах с точкой совпадает с метрикой $\epsilon^{\alpha\beta}$ в спинорных индексах без точек.

Метрика остается инвариантной при поворотах спиноров. Действительно, справедливо соотношение изометрии:

$$\hat R_S^{\mathrm{T}}\hat\epsilon\hat R_S = -\hat R_S^{\mathrm{T}}\hat\epsilon^{-1}\hat R_S = \hat\epsilon\left(\hat\epsilon\hat R_S^{\mathrm{T}}\hat\epsilon^{-1}\right)\hat R_S = \hat\epsilon\hat R_S^\dagger\hat R_S = \hat\epsilon,$$

где мы воспользовались тождеством (9.25). Группа инвариантности спинорной метрики с $\det\hat R_S = 1$ называется специальной унитарной группой на двухкомпонентных спинорах: $SU(2)$. Это трехпараметрическая группа.

Мы исследовали алгебру генераторов группы при построении поворотов спиноров. Эта алгебра совпадает с алгеброй генераторов группы поворотов трехмерного евклидова пространства $SO(3)$. Тем не менее, сами группы отличаются, так как в $SU(2)$ допустимы и полуцелые собственные значения генератора s_z, а в $SO(3)$ - только целые значения s_z. Это особенно ярко проявляется при проведенном выше рассмотрении поворота на угол 2π: для спиноров этот поворот дает фактор -1, а для бозонов, полей с целым значением спина, - фактор $+1$. Другими словами, ядро гомоморфизма $SU(2)$ на $SO(3)$, т.е. праобраз единицы, - это дискретная группа $\mathbb{Z}_2$, состоящая из 2х элементов $\{1,-1\}$. В математике имеет место утверждение: представления алгебры Ли реализуют представления универсальной накрывающей группы. В рассмотренном случае, исходная группа Ли - группа поворотов 3-мерного евклидова пространства $SO(3)$, представления

её алгебры эо(3) реализуют представления группы, которая является универсальной накрывающей группой для $SO(3)$, это - группа $SU(2)$. Физический смысл этого утверждения мы указали: для представлений группы $SU(2)$, универсальной накрывающей группы $SO(3)$, допустимы полуцелые значения спина, в отличие от представлений самой группы $SO(3)$, для которой допустимы только целые значения сiлина.

Само существование полей с полуцелым спином возможно, но оно не следует, вообще говоря, из группы поворотов евклидова пространства. Факт такого существования - экспериментальный. Подчеркнем, что спинорная метрика задает инвариант

$$\psi \cdot \psi = \psi_\alpha \epsilon^{\alpha\beta} \psi_\beta = \psi_{(1)}\psi_{(2)} - \psi_{(2)}\psi_{(1)},$$

и это инвариант обратился бы в нуль [1], если бы спиноры описывались обычными комплексными числами! Этот факт напрямую связан с тем, что спиноры - частный случай фермионов с полуцелым спином, для которых имеет место принцип запрета Паули. Из принципа запрета Паули, как мы узнаем (см. стр. 158 раздел 9.3), следует, что перестановка наблюдаемых параметров тождественных фермионов, в данном случае, перестановка номеров поляризации (проекции спина на ось z) в амплитуде вероятности должна сопровождаться сменой знака амплитуды. В частности, следует положить, что

$$\psi_{(1)}\psi_{(2)} = -\psi_{(2)}\psi_{(1)},$$

что в математике называют алгеброй Грассмана, а сами числа с такими свойствами - грассмановыми переменными. Укажем лишь, что в релятивистской теории устанвливается связь спина со статистикой: собственное значение оператора перестановок тождественных частиц равно $+1$ для частиц с целым спином (бозонов) и -1 для для частиц с полуцелым спинов (фермионов). Тогда становится понятным, почему метрика пространства как инвариантная квадратичная форма на вещественных векторах симметрична, а метрика спинорного пространства на грассмановых спинорах антисимметрична.

Как догадаться про это?

4.5.4 Connection of Spin with Statistics (!!????)

Подробно обсудим связь спина со статистикой.

Суть

Доказательство на пальцах

(?? как это на интуитивном уровне доказать?)

Типичная теория

РассМоТриМ ДВа тождественных фермиона.
Их волновая функция -

$$\left\langle \boldsymbol{r}_1, \theta^\alpha_{(1)}, n_1; \boldsymbol{r}_2, \theta^\beta_{(2)}, n_2 | \Psi \right\rangle = \psi^{(n_1,n_2)}_{\alpha\beta}\left(\boldsymbol{r}_1, \boldsymbol{r}_2\right)$$

где мы указали возможные многомерные квантовые числа (n_1, n_2), не связанные со спинорНыми характеристикам и.

После поворота на угол 2π координаты первой частицы r_1 и ее

$$\psi_{\alpha\beta}^{(n_1,n_2)}\left(\boldsymbol{r}_1,\boldsymbol{r}_2\right)\overset{\mathcal{R}_1(2\pi)}{\longrightarrow}\psi_{\alpha\beta}^{\mathcal{R}_1(n_1,n_2)}\left(\boldsymbol{r}_1,\boldsymbol{r}_2\right)=-\psi_{\alpha\beta}\left(\boldsymbol{r}_1,\boldsymbol{r}_2\right)$$

Подобное отличие в фазе волновой функции фермионов после вращения на угол 2π мо-
си туацию, когда квантовые числа двух ферм ионов тождествен но совпадают:

$$\boldsymbol{r}_1=\boldsymbol{r}_2=\boldsymbol{r},\quad \theta_{(1)}^{\alpha}=\theta_{(2)}^{\beta}=\theta^1,\quad n_1=n_2=n$$

т.е., Другим и словами, поместим тождественные частицы с одним и тем же набором знаЧений наблюдаемых величин в одну точку пространства.

В полной аналогии с выводом ДОПустимых значений квантованного орбитального момента потребуем выполнение следующего принци па: если состояния каждой из двух тождественных частиц не отличи мы, то вращение одной из них на угол 2π не наблюдаемо, т.е.

Должно приводить к тождественному преобразован ию состояния.

По сути, речь идет о вращении одной части цы отгиосителъио сТН, В одн ой точке), то такое вращение не имеет физического смысла, т.е.

не наблюдаемо.

Следовательно, исходная волновая функция

$$\psi_{11}^{(n,n)}(\boldsymbol{r},\boldsymbol{r})$$

ДОЛжна тождественно совпадать с волновой фун кцией после вращения координат одной из Частиц на угол 2π :

$$\psi_{11}^{(n,n)}\left(\mathbf{r},\mathbf{r}'\right)=-\psi_{11}^{(n,n)}(\mathbf{r},\boldsymbol{r})\equiv 0$$

Что ДОСтигается только в случае равенства нулю волновой функци и тождественных фер- . Этот прин цип автоматически удовлетворяется, если волновую функцию тождественных

$$\psi_{\alpha\beta}^{A(n_1,n_2)}\left(\boldsymbol{r}_1,\boldsymbol{r}_2\right)=\frac{1}{\sqrt{2}}\left\{\psi_{\alpha\beta}^{(n_1,n_2)}\left(\boldsymbol{r}_1,\boldsymbol{r}_2\right)-\psi_{\beta\alpha}^{(n_2,n_1)}\left(\boldsymbol{r}_2,\boldsymbol{r}_1\right)\right\}$$

так как она обращается в нуль, если квантовые состояния фермионов тождественны

А нтисим метризованная волновая функция Двух фермионов являет собой пример обшего принципа, возникающего в Квантовой механике с тождествен ными частицами.

В самом деле, физическая система из тождествен ных частиц не изменится, если поменять местами пару этих части ц.

В квантовой механике это утвержден ие означает, что состояиие системъе

$$\left|\Psi:\{Q_1,Q_2,...\}\right\rangle=\lambda\left|\Psi:\{Q_2,Q_1,...\}\right\rangle,\quad |\lambda|=1$$

где $\{Q_1,Q_2,...\}$ -полный набор наблюдаемых для частиц $\{1,2,...\}$.В этом уравнени и MbI ТребуеМ, Чтобы при перестановке квантовых чисел первой и второй частиц вектор состояния остался прежним с точ ностью до фазового множителя (норм ировка остается без.

изменения).

Если ввести оператор перестановок

$$\hat{\delta}_{1\leftrightarrow 2}\left|\Psi:\{Q_1,Q_2,...\}\right\rangle=\left|\Psi:\{Q_2,Q_1,...\}\right\rangle$$

то (9.28) есть ни что и ное, как уравнение на собствен ные значения для.

Двукратное при- менение перестановки возвращает систему к исходному состоян ию:

$$\hat{\mathcal{S}}\hat{\mathcal{S}} = 1$$

ОТКуда немедлен но следует, что спектр собствен ных значений оператора перестановок тождественных частиц

$$\lambda^2 = 1 \leftrightarrow \quad \lambda = \pm 1$$

Поскольку перестановки не изменяют н ИКаких наблюдаем ых харак тери стик систем ы ТОЖДественных частиц, оператор перестановок ком мутирует со всеми наблюдаемы ми

$$[\hat{\mathrm{S}}, \hat{H}] = [\hat{\mathrm{S}}, \hat{\boldsymbol{p}}] = [\hat{\mathrm{s}}, \hat{\boldsymbol{j}}] = ... = 0$$

Числа двух тождественных частиц совпадают.

Как мы видели, это имеет место Для ферм иОНОВ -частиц с полуцелым сп ином.

В этом случае

$$\lambda = e^{2\pi i s}$$

где s -значение сп ина каждой из тождественных частиц.

Эта форм ула, полученная для Полуцелых значений спина частиц, остается справедлива и для целых значен ий спина, Т.е.

Для бозонов, которые, таким образом, и меют сим метризованные по перестановкам волновые функции.

Именно, в природе не наблюдаются псевдо-бозоны целого спина с антисимметричным и по перестановкам волновыми функциями.

Тем не менее, поля так их частиц используются Для вспомогательных целей в квантовой теории поля для наиболее наглядной форм ули ровк и некоторых прин ципов сим метрии.

Поля псевдо-бозонов называют "гостам и" (от ан глийского ghost, Что значит "дух") или просто "духами".

При этом, ОДн ако, полагаЮт, что число духов в начальном и конечном состоянии равно нулю, т.е.

В полный набор наблюдаемых включают число ДУхов, тождественно равн ое нулю.

Подчеркнем, что рассмотренная связь спина со стати стикой возникла благодаря пространственной вращательной симметрии для спиноров, т.е.

благодаря группе $SU(2)$. ОДнако это не знач ит, что присутствие какой-либо Другой си мметри и со спинорами в группе $SU(2)$ так же неми нуемо при ведет к антисимметризации волновых функций.

Например, в стандартную модель взаимодействий элементарн ых части ц включено скалярное, а следоВательно, бозонн ое, поле со спином 0, которое является спи нором по калибровочной гр уппе $SU(2)$. Как мы показали, нали чие калибровоч ной группы сим метрии отвечает сохранени ю Заряда, который в данном случае - заряд частицы в слабом взаимодействии.

Эта калиброВОЧная группа никак не связана с пространственными вращениям и, и поэтом у она не означает введения каких-либо дополни тельн ых ограни чений на волновую функци ю, связанн ых с сим метрией по перестановкам.

Такие группы, не связанные с вращениям и пространства, называются группами внутрен ней си мм етри и.

Генераторы таких гр упп, следовательно, Коммутируют с генераторами вращений и трансляций

Элементарное объяснение принципа Паули

(потом еще раз посмотрю.)

Принцип тождественности частиц на языке волновых функций означает, что волновые функции системы частиц, получающиеся друг из друга перестановкой пар одинаковых частиц, могут отличаться только несущественным множителем e^{if}, где f -вещественное число.

Добавление этого множителя не меняет ни плотности вероятности $|\psi|^2$ обнаружения частиц, ни средних значений физических величин.

Если сделать перестановку частицы еще раз, то получится функция, отличающаяся от исходной множителем e^{2if}.

Так как при этом система возвращается в исходное состояние, то $e^{2if} = 1$ и $e^{if} = \pm 1$.

Следовательно, перестановка пары частиц местами либо оставляет волновую функцию неизменной, либо меняет ее знак.

обзор применений принципа паули

отсылки в разные места, где он играет важную роль.
подробно про все это!
в нейтронных звездах
в квантовом ферми газе

Как догадаться про это?

4.5.5 Generalization of Spin to Spinors

Обсудим спиноры как обобщение спина. Подробно спиноры обсудим или в дополнениях или в теории поля.

4.5.6 Other About Spin

О бытовых аналогиях (?)

(укажу их потом тут.)

О моделях со спинами

О моделях со спинами

(????)

О твердотельных моделях со спинами

(тут их укажу, их полно)

пример: Дублетная структура спектральных линий натрия

итак, подумаем, если у нас атом излучает две близкие спектральные линии, как это можно объяснить?

(попробовать по бору это сделать)
и как это мы объясним????

пример: периодичность таблицы менделеева

(потом как-то с помощью спина это нужно объяснить. я ведь теоретик.
так что нужно думать над этой теорией.
как ее построить? как очевидно может быть, что это именно спин спасет ситуацию?)

О спиновой метрике (???)

(потом мб добавлю этот раздел, пока хз, нужен ли.)

4.5.7 1. Spin

1.1. Spin operators.

So far we have been tacitly assuming that the Hilbert space for a quantum particle is $\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{x})$. Based on this assumption, in Section 5.1 of Chapter 3 we have found the energy levels of the hydrogen atom. In particular, in the ground state the third component M_3 of the quantum angular momentum operator M has eigenvalue 0 . However, the famous Stern-Gerlach experiment has shown that the electron in the hydrogen atom also has a "magnetic angular momentum", whose third component in the ground state may take two values which differ by a sign. Therefore in addition to the "mechanical angular momentum" operator $\boldsymbol{M}$ with components M_1, M_2, M_3, the electron also has the "internal angular momentum" operator S with components S_1, S_2, S_3, called spin. The spin describes internal degrees of freedom of the electron and is independent of its position in the space [1]. The Hilbert space of states of the electron is $\mathscr{H}_S = \mathscr{H} \otimes \mathbb{C}^2$, i.e., it has twice as many states than a spinless particle. The Hilbert space $\mathscr{H}_S$ consists of two-component vector-valued functions on $\mathbb{R}^3$,

$$\Psi = \begin{pmatrix} \psi_1(\boldsymbol{x}) \\ \psi_2(\boldsymbol{x}) \end{pmatrix} \in \mathscr{H}_S,$$

where

$$\|\Psi\|^2 = \int_{\mathbb{R}^3} |\psi_1(\boldsymbol{x})|^2 \, d^3\boldsymbol{x} + \int_{\mathbb{R}^3} |\psi_2(\boldsymbol{x})|^2 \, d^3\boldsymbol{x} < \infty.$$

To every observable A in $\mathscr{H}$ there corresponds an observable $A \otimes I_2$ in $\mathscr{H}_S$, given by the 2×2 block-diagonal matrix $\begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix}$. Observables of the form $I \otimes S$, where I is the identity operator in $\mathscr{H}$ and S is a self-adjoint operator in $\mathbb{C}^2$, describe the inner degrees of freedom and commute with all observables $A \otimes I_2$. The complete set of the observables in $\mathscr{H}_S$ consists of the operators $Q_1 \otimes I_2, Q_2 \otimes I_2, Q_3 \otimes I_2$ and $I \otimes S_1, I \otimes S_2, I \otimes S_3$, where Q_j are coordinate operators, and S_j are spin operators - traceless self-adjoint operators in $\mathbb{C}^2$, satisfying the same commutation relations as the quantum operators of the angular momentum,

$$[S_1, S_2] = i\hbar S_3, \quad [S_2, S_3] = i\hbar S_1, \quad [S_3, S_1] = i\hbar S_2$$

In terms of the standard basis $e_1 = \binom{1}{0}, e_2 = \binom{0}{1}$ of $\mathbb{C}^2, S_j = \frac{\hbar}{2}\sigma_j, j = 1, 2, 3$, where σ_j are the so-called Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

which are commonly used in physics. It is also convenient to represent $\Psi \in \mathscr{H}_S$ as a function $\psi(\boldsymbol{x}, \sigma)$ of two variables, where $\boldsymbol{x} \in \mathbb{R}^3$ and σ takes two values $\frac{1}{2}$ and $-\frac{1}{2}$, by setting

[01] The spin is a pure quantum effect which is absent in classical mechanics.

$\psi\left(\boldsymbol{x}, \frac{1}{2}\right) = \psi_1(\boldsymbol{x})$ and $\psi\left(\boldsymbol{x}, -\frac{1}{2}\right) = \psi_2(\boldsymbol{x})$. Every function $\psi(\boldsymbol{x}, \sigma)$ is a finite linear combination of the functions $\psi(\boldsymbol{x})\chi(\sigma)$ the decomposable elements of the tensor product $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$. Here we are identifying $\mathbb{C}^2$ with the complex vector space of functions $\chi : \left\{-\frac{1}{2}, \frac{1}{2}\right\} \to \mathbb{C}$ by assigning to the standard basis e_1, e_2 the functions χ_1, χ_2, defined by $\chi_1\left(\frac{1}{2}\right) = 1, \chi_1\left(-\frac{1}{2}\right) = 0$ and $\chi_2\left(\frac{1}{2}\right) = 0, \chi_2\left(-\frac{1}{2}\right) = 1$. This identification is also commonly used in physics.

In this notation the operator S_3 becomes a multiplication by $\hbar\sigma$ operator,

$$S_3\psi(\boldsymbol{x}, \sigma) = \hbar\sigma\psi(\boldsymbol{x}, \sigma)$$

and

$$S_1\psi(\boldsymbol{x}, \sigma) = \hbar|\sigma|\psi(\boldsymbol{x}, -\sigma), \quad S_2\psi(\boldsymbol{x}, \sigma) = -i\hbar\sigma\psi(\boldsymbol{x}, -\sigma)$$

Here and in what follows we will always assume that spin operators act only on the variable σ, and will often write S_j instead of $I \otimes S_j$. The operator $\boldsymbol{S}^2 = S_1^2 + S_2^2 + S_3^2$ is called the square of the total spin operator, and $\boldsymbol{S}^2 = \hbar^2 s(s+1)I_2$, where $s = |\sigma| = \frac{1}{2}$ is a total spin. In physics terminology, the electron has spin $\frac{1}{2}$.

1.2. Spin and representation theory of SU(2)

Mathematical interpretation of spin is provided by the representation theory of the Lie algebra $\mathfrak{su}(2)$, discussed in Section 3.2 of Chapter 3. Namely, let

$$A_1 = \frac{i}{2}\sigma_1, \quad A_2 = -\frac{i}{2}\sigma_2, \quad A_3 = -\frac{i}{2}\sigma_3$$

be the standard basis of the Lie algebra $\mathfrak{su}(2) - 2 \times 2$ traceless skewHermitian matrices satisfying commutation relations

$$[A_1, A_2] = A_3, \quad [A_2, A_3] = A_1, \quad [A_3, A_1] = A_2$$

and let $\rho_{\frac{1}{2}}$ be the two-dimensional (fundamental) representation of $\mathfrak{su}(2)$ in $V_{\frac{1}{2}} \simeq \mathbb{C}^2$. The spin operators are given by

$$S_j = i\hbar\rho_{\frac{1}{2}}(A_j), \quad j = 1, 2, 3,$$

and $\rho_{\frac{1}{2}}$ is called the representation of spin $\frac{1}{2}$. In general, representation ρ_s in the $2s+1$-dimensional complex vector space V_s is called the representation of spin $s \in \frac{1}{2}\mathbb{Z}_{\geq 0}$. The action of operators $T_j = i\rho_s(A_j)$ in V_s is described by formulas (3.10)-(3.12) in Section 3.2 of Chapter 3 (where l is replaced by s). There is another explicit realization of the representation ρ_s in the vector space $\mathscr{P}_s$ of polynomials $f(z)$ of degree not greater than $2s$. Namely, the mapping

$$e_{sm} \mapsto \frac{z^{s+m}}{\sqrt{(s+m)!(s-m)!}}, \quad m = -s, -s+1, ..., s-1, s$$

establishes the isomorphism between the vector space V_s with the inner product determined by the orthonormal basis e_{sm}, and the vector space $\mathscr{P}_s$ with the inner product

$$(f, g) = \frac{(2s+1)!}{\pi}\int_{\mathbb{C}} \frac{f(z)\overline{g(z)}}{(1+|z|^2)^{2s+2}} d^2z, \quad f, g \in \mathscr{P}_s \tag{1.1}$$

Corresponding operators $T_j = i\rho_s(A_j)$ in $\mathscr{P}_s$ are given by

$$T_1 - iT_2 = \frac{d}{dz}, \quad T_1 + iT_2 = z^2\frac{d}{dz} - 2sz, \quad T_3 = z\frac{d}{dz} - s \tag{1.2}$$

It is easy to verify that T_1, T_2, T_3 are Hermitian operators with respect to the inner product (1.1). Representation ρ_s of the Lie algebra $\mathfrak{su}(2)$ is integrable, $\rho_s = dR_s$, where R_s is an irreducible unitary representation of the Lie group SU(2), defined by

$$R_s(g)(f)(z) = (\bar{\beta}z + \alpha)^{2s} f\left(\frac{\bar{\alpha}z - \beta}{\bar{\beta}z + \alpha}\right), \quad g = \begin{pmatrix} \alpha & \beta \\ -\bar{\beta} & \bar{\alpha} \end{pmatrix} \in \mathrm{SU}(2), \quad f \in \mathscr{P}_s.$$

Remark. The spin $\frac{1}{2}$ representation $R_{\frac{1}{2}}$ in $\mathbb{C}^2$ can also be explicitly described as

$$R_{\frac{1}{2}}(g)\boldsymbol{z} = \begin{pmatrix} \alpha & \beta \\ -\bar{\beta} & \bar{\alpha} \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}, \quad \boldsymbol{z} = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \in \mathbb{C}^2$$

and is called the fundamental representation.

Remark. Representation R_s of SU(2) can be lifted to a family of representations of the general unitary group U(2) acting in the same vector space $\mathscr{P}_s$. Namely, every $g \in \mathrm{U}(2)$ can be written as $g = \alpha g_0$, where $\alpha^2 = \det g$ and is determined up to a sign, and $g_0 \in \mathrm{SU}(2)$. Then for every integer l with the property that $2s + l$ is even, the formula

$$R_{l,s}(g) = \alpha^l R_s(g_0)$$

defines an irreducible unitary representation of U(2) in $\mathscr{P}_s$. The condition that $\frac{l}{2} + s$ is an integer ensures that $R_{l,s}$ does not depend on the choice of a sign in the definition of α. The representation $R_{l,s}$ is the highest weight representation of U(2) with the dominant weights $\lambda_1 = \frac{l}{2} + s \geq \lambda_2 = \frac{l}{2} - s$, $\lambda_1 + \lambda_2 = l$. We will denote the corresponding U(2)-module as $V_{\lambda,l}$, where $\lambda = (\lambda_1, \lambda_2)$ is a dominant weight with $\lambda_1 + \lambda_2 = l$. As an SU(2)-module, $V_{\lambda,l} = V_s$, where $s = \frac{1}{2}(\lambda_1 - \lambda_2)$.

Returning to the basic principles of quantum mechanics, formulated in Section 1 of Chapter 2, we now extend the first postulate A1 to the case of particles with spin.

A10 (Particles with Spin). The Hilbert space of states for a quantum particle of a spin $s \in \left\{0, \frac{1}{2}, 1, \frac{3}{2}, ...\right\}$ is

$$\mathscr{H}_S = L^2\left(\mathbb{R}^3\right) \otimes V_s$$

where V_s is a $2s + 1$-dimensional complex vector space of the irreducible representation R_s of the Lie group SU(2) of spin s. The spin operators $\boldsymbol{S} = (S_1, S_2, S_3)$ are given by

$$S_j = i\hbar\rho_s(A_j), \quad j = 1, 2, 3$$

where A_1, A_2, A_3 are standard generators of the Lie algebra $\mathfrak{su}(2)$ and $\rho_s = dR_s$ is the corresponding representation of $\mathfrak{su}(2)$ in V_s. Particles with integer spin are called bosons, and particles with half-integer spin are called fermions.

As in the case of spin $\frac{1}{2}$, it will be convenient to represent $\Psi \in \mathscr{H}_S$ as a function $\psi(\boldsymbol{x}, \sigma)$ of two variables, where $\boldsymbol{x} \in \mathbb{R}^3$ and the variable σ takes $2s+1$ values from the set $\{-s, -s+1, ..., s-1, s\}$. For a given σ, the function $\psi(\boldsymbol{x}, \sigma)$ is the k-th component, $k = s - \sigma + 1$, of the $2s + 1$-dimensional vector $\Psi(\boldsymbol{x})$. Every function $\psi(\boldsymbol{x}, \sigma)$ is a finite linear combination of the functions $\psi(\boldsymbol{x})\chi(\sigma)$ - the decomposable elements of the tensor product $L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2s+1}$, where we are identifying $\mathbb{C}^{2s+1}$ with the complex vector space of functions $\chi : \{-s, -s+1, ..., s-1, s\} \to \mathbb{C}$ by assigning to the elements e_k of the standard basis $e_1, ..., e_{2s+1}$ the functions χ_k, defined by $\chi_k(s + 1 - k) = 1$ and being 0 otherwise.

The complete set of observables for a quantum particle of spin s consists of position operators $Q_1 \otimes I_{2s+1}, Q_2 \otimes I_{2s+1}, Q_3 \otimes I_{2s+1}$, where I_{2s+1} is the identity operator in V_s, and spin operators $I \otimes S_1, I \otimes S_2, I \otimes S_3$. The total angular momentum operators $\boldsymbol{J} = (J_1, J_2, J_3)$ in $\mathscr{H}_S$ are self-adjoint operators in $\mathscr{H}_S$ given by

$$\boldsymbol{J} = \boldsymbol{M} \otimes I_{2s+1} + I \otimes \boldsymbol{S}$$

They satisfy the same commutation relations as the spin operators,

$$[J_1, J_2] = i\hbar J_3, \quad [J_2, J_3] = i\hbar J_1, \quad [J_3, J_1] = i\hbar J_2$$

As angular momentum operators $\boldsymbol{M}$ (see Lemma 3.1 in Section 3.2 of Chapter 3), the total angular momentum operators $\boldsymbol{J}$ are associated with the unitary representation of the Lie group SU(2) in the Hilbert space $\mathscr{H}_S = L^2(\mathbb{R}^3, d^3\boldsymbol{x}) \otimes V_s$. Namely, let R be the unitary representation of SU(2) in $\mathscr{H} = L^2(\mathbb{R}^3, d^3x)$ corresponding to the adjoint representation of SU(2) in $\mathfrak{su}(2) \simeq \mathbb{R}^3$,

$$(R(g)\psi)(\boldsymbol{x}) = \psi\left(\operatorname{Ad} g^{-1}\boldsymbol{x}\right), \quad g \in \mathrm{SU}(2), \quad \psi \in \mathscr{H}$$

where

$$(\operatorname{Ad} g\boldsymbol{x}) \cdot \boldsymbol{\sigma} = g(\boldsymbol{x} \cdot \boldsymbol{\sigma})g^{-1}, \quad \boldsymbol{x} \cdot \boldsymbol{\sigma} = x_1\sigma_1 + x_2\sigma_2 + x_3\sigma_3$$

Lemma 1.1. We have

$$(R \otimes R_S)\left(e^{a_1A_1 + a_2A_2 + a_3A_3}\right) = e^{-\frac{i}{\hbar}(a_1J_1 + a_2J_2 + a_3J_3)}$$

where $\boldsymbol{a} = (a_1, a_2, a_3) \in \mathbb{R}^3$.

Problem 1.1. Derive formulas (1.2) and show that operators T_1, T_2, T_3 are Hermitian with respect to the inner product (1.1).

Problem 1.2. Prove Lemma 1.1.

4.5.8 3. System of Identical Particles

Consider the quantum system of N particles of spins $s_1, ..., s_N$. According to the basic principles of quantum mechanics, the Hilbert space of states of the system is given by

$$\mathscr{H}_N = \mathscr{H}_{S_1} \otimes \cdots \otimes \mathscr{H}_{S_N} = \underbrace{L^2\left(\mathbb{R}^3\right) \otimes \cdots \otimes L^2\left(\mathbb{R}^3\right)}_{N} \otimes V_{s_1} \otimes \cdots \otimes V_{s_N}$$

In terms of the variables $\boldsymbol{\xi}_i = (\boldsymbol{x}_i, \sigma_i)$, where $\boldsymbol{x}_i \in \mathbb{R}^3$ and $\sigma_i \in \{-s_i, -s_i + 1, ..., s_i - 1, s_i\}$, the total wave function of the system can be written as $\Phi(\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_N)$. The total wave function is a finite linear combination of the product functions

$$\Phi(\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_N) = \Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)\,\chi(\sigma_1, ..., \sigma_N)$$

where $\Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N) \in L^2\left(\mathbb{R}^{3N}\right)$ is a coordinate part, and $\chi(\sigma_1, ..., \sigma_N)$ is a spin part of the total wave function. The spin part, in accordance with the tensor product structure $V_{s_1} \otimes \cdots \otimes V_{s_N}$, is a finite linear combination of the products $\chi_{k_1}(\sigma_1) ... \chi_{k_N}(\sigma_N)$ of functions χ_k, defined in Section 1.

The Hamiltonian of the system of N-particles (without the spin interaction) in the coordinate representation has the form

$$H_N = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i}\Delta_i + \sum_{i=1}^{N} V_i(\boldsymbol{x}_i) + \sum_{1 \le i < k \le N} V_{ik}(\boldsymbol{x}_i - \boldsymbol{x}_k),$$

where the first term is the operator of kinetic energy of the system of N particles, the second term describes the interaction of the particles with the external field, and the last term

describes their pair-wise interaction. Note that though the Hamiltonian H_N acts only on the coordinate part $\Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)$ of the total wave function, the physical properties of the system do depend on the spins of the particles.

3.1. The symmetrization postulate. For the system of N identical particles of mass m and spin s the corresponding Hilbert space is

$$\mathscr{H}_N = L^2\left(\mathbb{R}^{3N}\right) \otimes V_s^{\otimes N} \tag{3.1}$$

The irreducible representation R_s of the Lie group $\mathrm{SU}(2)$ in the vector space V_s naturally defines a representation $R_s^{\otimes N}$ in $V_s^{\otimes N}$,

$$R_s^{\otimes N}(g)\,(v_1 \otimes \cdots \otimes v_N) = R_s(g)v_1 \otimes \cdots \otimes R_s(g)v_N, \quad g \in \mathrm{SU}(2)$$

The corresponding representation $\rho_s^{\otimes N}$ of the Lie algebra $\mathfrak{su}(2)$ is given by

$$\rho_s^{\otimes N}(x)\,(v_1 \otimes \cdots \otimes v_N) = \sum_{k=1}^{N} v_1 \otimes \cdots \otimes \rho_s(x)v_k \otimes \cdots \otimes v_N, \quad x \in \mathfrak{su}(2).$$

The total spin operators $\boldsymbol{S} = (S_1, S_2, S_3)$ of the system of N identical particles are given by

$$S_j = i\hbar\rho_s^{\otimes N}(A_j) = \sum_{k=1}^{N} S_j^{(k)}, \quad j = 1, 2, 3 \tag{3.2}$$

Here $S_j^{(k)} = I_{2s+1} \otimes \cdots \otimes i\hbar\rho_s(A_j) \otimes \cdots \otimes I_{2s+1}$ are the spin operators of the k-th particle; they act non-trivially only in the k-th factor of the tensor product $V_s^{\otimes N}$.

Representations $R_s^{\otimes N}$ and $\rho_s^{\otimes N}$ are reducible and contain all representations V_l with spins $l \in \frac{1}{2}\mathbb{Z}_{\geq 0}$ such that $sN - l$ are non-negative integers. Indeed, the square S^2 of the total spin operator has the form

$$S^2 = S_1^2 + S_2^2 + S_3^2 = S_-S_+ + S_3(S_3 + I)$$

where $S_\pm = S_1 \pm iS_2$ and I here is the identity operator in $V_s^{\otimes N}$. It is easy to see from (3.2) that the eigenvalues of the operator S_3 are $-\hbar sN$, $\hbar(-sN+1), ..., \hbar(sN-1), \hbar sN$. Now by Schur's lemma, restriction of S^2 to the irreducible representation V_l is $\hbar^2 l(l+1)$ times the identity operator in V_l. Since V_l contains a highest weight vector which is annihilated by the operator $S_+$and is an eigenvector of the operator S_3 with eigenvalue $\hbar l$, we conclude that $V_s^{\otimes N}$ contains all irreducible representations with spins $l \in \frac{1}{2}\mathbb{Z}_{\geq 0}$ such that $sN - l$ are non-negative integers. The problem of determining the multiplicities with which representations V_l appear in the decomposition $V_s^{\otimes N}$ into the direct sum of irreducible representations will be discussed below. It plays a fundamental role in classifying the energy levels of the system of N identical particles of spin s.

There is also a natural action of the symmetric group Sym_N on N elements on $\mathscr{H}_N$, given by

$$P_\pi\Phi(\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_N) = \Phi\left(\boldsymbol{\xi}_{\pi^{-1}(1)}, ..., \boldsymbol{\xi}_{\pi^{-1}(N)}\right), \quad \pi \in \mathrm{Sym}_N.$$

The corresponding Hamiltonian in this case has the form

$$H_N = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_i + \sum_{i=1}^{N} V_{\mathrm{ext}}(\boldsymbol{x}_i) + \sum_{1 \leq i < k \leq N} V_{\mathrm{int}}(\boldsymbol{x}_i - \boldsymbol{x}_k), \tag{3.3}$$

and commutes with the Sym_N-action:

$$[H_N, P_\pi] = 0 \quad \text{for all} \quad \pi \in \mathrm{Sym}_N$$

Thus the operator H_N can be restricted to the Sym_N-invariant subspaces of $\mathscr{H}$, in particular to the subspace $\mathscr{H}_N^{(\mathrm{S})}$ of totally symmetric functions $\Phi(\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_N)$,

$$P_\pi \Phi = \Phi \quad \text{for all} \quad \pi \in \mathrm{Sym}_N$$

and to the subspace $\mathscr{H}_N^{(\mathrm{A})}$ of totally anti-symmetric functions $\Phi(\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_N)$,

$$P_\pi \Phi = (-1)^{\varepsilon(\pi)} \Phi \quad \text{for all} \quad \pi \in \mathrm{Sym}_N$$

where $\varepsilon(\pi)$ is the parity of a permutation π.

In classical mechanics, it is possible to label the identical particles (say by the integers $1, 2, ..., N$), and to trace the trajectory of each labeled particle separately. It follows from the Heisenberg uncertainty relations that in quantum mechanics it is impossible to trace the time evolution of labeled particles separately. In other words, in quantum mechanics identical particles are truly "indistinguishable", so that the Hilbert space (3.1) contains "too many states". It is another postulate of quantum mechanics which specifies "correct" Hilbert space of states for the system of identical particles.

A11 (The Symmetrization Postulate). The Hilbert space of states for the system of N identical particles of spin s is the totally symmetric subspace $\mathscr{H}_N^{(\mathrm{S})}$ of the N-fold tensor product $\left(L^2(\mathbb{R}^3) \otimes V_s\right)^{\otimes N}$ for the case of bosons (particles with integer spin), and is the totally anti-symmetric subspace $\mathscr{H}_N^{(\mathrm{A})}$ for the case of fermions (particles with half-integer spin).

Remark. The symmetrization postulate implies the Pauli exclusion principle, which states that no two fermions can occupy the same state. The Pauli exclusion principle is fundamental for atomic and molecular physics, and for the whole body of chemistry.

For the case of identical particles of spin 0 it follows from the symmetrization postulate that the corresponding Hilbert space $\mathscr{H}_N^{(\mathrm{S})}$ is the subspace of all totally symmetric functions $\Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)$ in $L^2\left(\mathbb{R}^{3N}\right)$, and in order to find the energy levels of the system, one needs to solve the Schrdinger equation

$$H_N \Psi = E_N \Psi \tag{3.4}$$

only in the totally symmetric subspace $\mathscr{H}_N^{(\mathrm{S})}$ of $\mathscr{H}_N$. Solutions of the eigenvalue problem (3.4) that do not belong to this subspace have no physical interpretation.

For the spin $\frac{1}{2}$ particles the situation is different: the symmetry properties of the coordinate part of the total wave function depend on the symmetry properties of the corresponding spin part. Consider first the simple example of a system of two electrons. In this case we have the direct sum decomposition of Hilbert spaces,

$$\mathscr{H}_2 = \mathscr{H}_2^{(\mathrm{S})} \oplus \mathscr{H}_2^{(\mathrm{A})},$$

which immediately follows from the representation

$$\Phi(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2) = \frac{1}{2}\left(\Phi(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2) + \Phi(\boldsymbol{\xi}_2, \boldsymbol{\xi}_1)\right) + \frac{1}{2}\left(\Phi(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2) - \Phi(\boldsymbol{\xi}_2, \boldsymbol{\xi}_1)\right).$$

Using the identity

$$\begin{aligned}
&\Psi(\boldsymbol{x}_1, \boldsymbol{x}_2)\chi(\sigma_1, \sigma_2) - \Psi(\boldsymbol{x}_2, \boldsymbol{x}_1)\chi(\sigma_2, \sigma_1) \\
&= \frac{1}{2}\left(\Psi(\boldsymbol{x}_1, \boldsymbol{x}_2) + \Psi(\boldsymbol{x}_2, \boldsymbol{x}_1)\right)\left(\chi(\sigma_1, \sigma_2) - \chi(\sigma_2, \sigma_1)\right) \\
&+ \frac{1}{2}\left(\Psi(\boldsymbol{x}_1, \boldsymbol{x}_2) - \Psi(\boldsymbol{x}_2, \boldsymbol{x}_1)\right)\left(\chi(\sigma_1, \sigma_2) + \chi(\sigma_2, \sigma_1)\right),
\end{aligned}$$

we can represent $\mathscr{H}_2^{(\mathrm{A})}$ as a direct sum of Hilbert spaces

$$\mathscr{H}_2^{(\mathrm{A})} = \mathfrak{S}_0 \oplus \mathfrak{S}_1,$$

where

$$\mathfrak{S}_0 = \left(L^2\left(\mathbb{R}^3\right) \otimes L^2\left(\mathbb{R}^3\right)\right)^{(\mathrm{S})} \otimes \wedge^2\mathbb{C}^2$$

consists of finite linear combinations of the product functions $\Phi\left(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2\right) = \Psi\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right)\chi\left(\sigma_1, \sigma_2\right)$, where $\Psi\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right) \in L^2\left(\mathbb{R}^3\right) \otimes L^2\left(\mathbb{R}^3\right)$ is symmetric and $\chi\left(\sigma_1, \sigma_2\right) \in \wedge^2\mathbb{C}^2$ is anti-symmetric, and

$$\mathfrak{S}_1 = \left(L^2\left(\mathbb{R}^3\right) \otimes L^2\left(\mathbb{R}^3\right)\right)^{(\mathrm{A})} \otimes \mathrm{Sym}^2\,\mathbb{C}^2$$

consists of finite linear combinations of the product functions where $\Psi\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right)$ is anti-symmetric and $\chi\left(\sigma_1, \sigma_2\right)$ is symmetric. The vector space $\wedge^2\mathbb{C}^2$ is onedimensional and is spanned by the function χ_{00}, which corresponds to the vector

$$\frac{1}{\sqrt{2}}\left(e_1 \otimes e_2 - e_2 \otimes e_1\right) \in \mathbb{C}^2 \otimes \mathbb{C}^2$$

and the vector space $\mathrm{Sym}^2\,\mathbb{C}^2$ is three-dimensional and is spanned by the functions $\chi_{11}, \chi_{10}, \chi_{1-1}$, which correspond to the vectors

$$e_1 \otimes e_1, \quad \frac{1}{\sqrt{2}}\left(e_1 \otimes e_2 + e_2 \otimes e_1\right), \quad e_2 \otimes e_2 \in \mathbb{C}^2 \otimes \mathbb{C}^2$$

Comparing the decomposition

$$\mathbb{C}^2 \otimes \mathbb{C}^2 = \wedge^2\mathbb{C}^2 \oplus \mathrm{Sym}^2\,\mathbb{C}^2$$

with the Clebsch-Gordan decomposition

$$V_{\frac{1}{2}} \otimes V_{\frac{1}{2}} = V_0 \oplus V_1,$$

discussed in Section 3.2 of Chapter 3, we see that ${}^2\wedge^2\mathbb{C}^2 = V_0$ and $\mathrm{Sym}^2\,\mathbb{C}^2 = V_1$. In physics terminology, V_0 is the spin singlet space, and V_1 is the spin triplet space. We summarize the obtained results in the following statement.

Proposition 3.1. For a system of two identical particles of spin $\frac{1}{2}$ the total wave function of spin 0 has the form $\Psi\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right)\chi_{00}\left(\sigma_1, \sigma_2\right)$, where $\Psi\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right)$ is symmetric and satisfies the Schrdinger equation (3.4). The total wave function of spin 1 has the form $\Psi\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right)\chi_{1m}\left(\sigma_1, \sigma_2\right)$, where $m = -1, 0, 1$, and $\Psi\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right)$ is anti-symmetric and satisfies the Schrdinger equation (3.4).

Remark. The coordinate part $\Psi\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right)$ of the total wave function has the usual probabilistic interpretation. Thus for a simple example of a system of two electrons with $V_{\mathrm{int}}(\boldsymbol{x}) = 0$, the coordinate part of the total wave function has the form

$$\Psi\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right) = \frac{1}{\sqrt{2}}\left(\psi_1\left(\boldsymbol{x}_1\right)\psi_2\left(\boldsymbol{x}_2\right) \pm \psi_1\left(\boldsymbol{x}_2\right)\psi_2\left(\boldsymbol{x}_1\right)\right)$$

where $\psi_1(\boldsymbol{x})$ and $\psi_2(\boldsymbol{x})$ are two one-electron coordinate wave functions, the plus sign refers to the spin singlet state, and the minus sign refers to the spin triplet state. The corresponding probability density is

$$\begin{aligned}\left|\Psi\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right)\right|^2 d^3\boldsymbol{x}_1 d^3\boldsymbol{x}_2 = \tfrac{1}{2}\Big(&\left|\psi_1\left(\boldsymbol{x}_1\right)\right|^2\left|\psi_2\left(\boldsymbol{x}_2\right)\right|^2 + \left|\psi_1\left(\boldsymbol{x}_2\right)\right|^2\left|\psi_2\left(\boldsymbol{x}_1\right)\right|^2 \\ &\pm 2\,\mathrm{Re}\left(\psi_1\left(\boldsymbol{x}_1\right)\psi_2\left(\boldsymbol{x}_2\right)\overline{\psi_1\left(\boldsymbol{x}_2\right)\psi_2\left(\boldsymbol{x}_1\right)}\right)\Big) d^3\boldsymbol{x}_1 d^3\boldsymbol{x}_2\end{aligned}$$

where the last term is called the exchange energy. It follows from this formula that when two electrons are in a spin triplet state, there is a zero probability of finding them at the same point $\boldsymbol{x} \in \mathbb{R}^3$. However, when electrons are in a spin singlet state, there is a non-zero probability of finding them at the same point in space, which is due to the exchange energy.

Consider now the system of N particles of spin $\frac{1}{2}$. In this case the total wave function $\Phi(\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_N) \in \mathscr{H}_N^{(\mathrm{A})}$ satisfies

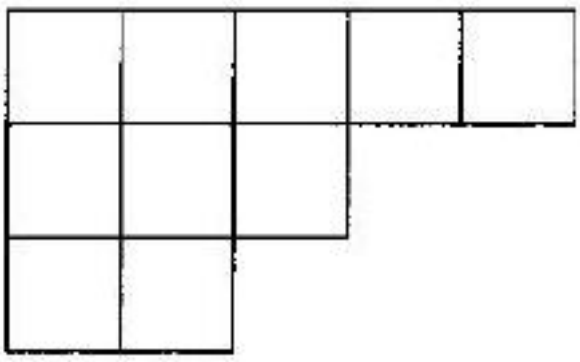
$$H_N \Phi = E_N \Phi \quad \text{and} \quad S^2 \Phi = s(s+1)\Phi \tag{3.5}$$

and describes the bound state with total spin s, where $\frac{1}{2}N - s$ is a nonnegative integer. It seems natural to assume that if one finds a coordinate wave function $\Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)$ satisfying (3.4), and a spin wave function $\chi(\sigma_1, ..., \sigma_N)$ which is the eigenfunction of S^2, then the total wave function $\Phi(\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_N)$ can be obtained by the anti-symmetrization:

$$\Phi(\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_N) = \sum_{\pi \in \mathrm{Sym}_N} (-1)^{\varepsilon(\pi)} \Psi\left(\boldsymbol{x}_{\pi(1)}, ..., \boldsymbol{x}_{\pi(N)}\right) \chi\left(\sigma_{\pi(1)}, ..., \sigma_{\pi(N)}\right)$$

However, it may happen that for a coordinate wave function $\Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)$ satisfying (3.4), the corresponding total wave function $\Phi(\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_N)$ is identically zero! The requirement that the total wave function $\boldsymbol{\Phi}(\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_N)$ is not identically zero determines admissible symmetry properties of the coordinate wave function $\Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)$, which are described by the irreducible representations of the symmetric group Sym_N.

3.2. Young diagrams and representation theory of Sym_N. The number of irreducible representations of the symmetric group Sym_N is the number of its conjugacy classes, which in turn is the number of partitions $\lambda = (\lambda_1, ..., \lambda_n)$ of $N : N = \lambda_1 + \cdots + \lambda_n$, where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 1$. Denote by $\mathrm{Par}(N)$ the set of all partitions of N. To each partition $\lambda \in \mathrm{Par}(N)$ there is an irreducible representation G_λ of Sym_N, constructed as follows. Let Y_λ be the Young diagram associated with $\lambda \in \mathrm{Par}(N)$ - a collection of N boxes arranged into n left-justified rows, with the first row containing λ_1 boxes, the second row containing λ_2 boxes, etc. Thus the diagram



corresponds to the partition $10 = 5 + 3 + 2$. A Young tableau A associated with the Young diagram Y_λ is an assignment of N integers $1, 2, ..., N$ to the N boxes such that each box gets a different integer; denote by $\mathfrak{T}_\lambda$ the set of all Young tableaux associated with the partition $\lambda \in \mathrm{Par}(N)$. A canonical Young tableau $A_\lambda \in \mathfrak{T}_\lambda$ is obtained by numbering the boxes consecutively along the rows from left to right. For a Young tableau $A \in \mathfrak{T}_\lambda$, say the canonical one, define two subgroups of Sym_N:

$$\mathrm{Row}(A) = \{\pi \in \mathrm{Sym}_N : \pi \text{ preserves the rows of } A\}$$
$$\mathrm{Col}(A) = \{\pi \in \mathrm{Sym}_N : \pi \text{ preserves the columns of } A\}$$

[02] This can also be verified directly by checking the action of total spin operators.

Now let $\mathfrak{A} = \mathbb{C}\mathbb{S}\curvearrowright\!\!\succ_N$ be the group algebra of Sym_N - a complex vector space with the basis $\{e_\pi\}_{\pi\in\mathrm{Sym}_N}$ and the multiplication map defined by $e_{\pi_1}\cdot e_{\pi_2} = e_{\pi_1\pi_2}$. Denote by R the regular representation of Sym_N in $\mathfrak{A}$, defined by

$$R(\pi)x = e_\pi \cdot x, \quad x \in \mathfrak{A}.$$

With a given Young tableau A one can associate two elements in the group algebra $\mathfrak{A}$: the row symmetrizer

$$\mathrm{R}_A = \sum_{\pi\in\mathrm{Row}(A)} \pi,$$

and the column anti-symmetrizer

$$\mathrm{C}_A = \sum_{\pi\in\mathrm{Col}(A)} (-1)^{\varepsilon(\pi)}\pi.$$

Define the Young symmetrizer by

$$\Pi_A = \mathrm{C}_A\mathrm{R}_A \in \mathfrak{A},$$

and consider the left Sym_N-module ${}^3G_\lambda = \mathfrak{A}\cdot\Pi_A$, and the representation $T_\lambda : \mathrm{Sym}_N \to \mathrm{End}\, G_\lambda$, where Sym_N acts by left multiplication. The following result is fundamental.

Theorem 3.1. Each T_λ is an irreducible representation of Sym_N, and representations T_λ and T_μ are not isomorphic if $\lambda \neq \mu$. The dimension of the representation T_λ is given by the Frobenius formula

$$d_\lambda = \frac{N!}{l_1!...l_n!}\prod_{i<j}(l_i - l_j), \quad l_i = \lambda_i + n - i, \quad i = 1, ..., n,$$

and $\Pi_A^2 = d_\lambda\Pi_A$. Every irreducible representation of Sym_N is isomorphic to the representation T_λ for some partition $\lambda \in \mathrm{Par}(N)$.

Remark. It follows from the representation theory of finite groups that

$$R = \bigoplus_{\lambda\in\mathrm{Par}(N)} d_\lambda G_\lambda \quad \left(\mathfrak{A} = \bigoplus_{\lambda\in\mathrm{Par}(N)} \mathrm{End}\ G_\lambda \text{ as algebras}\right),$$

so that

$$N! = \sum_{\lambda\in\mathrm{Par}(N)} d_\lambda^2.$$

There is another expression for dimensions d_λ as a product over the boxes of the Young diagram Y_λ, given by the so-called hook-length formula.

Remark. One can explicitly construct the bases in the subspaces G_λ by the following procedure. Let A be the standard Young tableau for a partition $\lambda \in \mathrm{Par}(N)$: a Young tableau with the condition that in each row of Y_λ, the numbers in the boxes are strictly increasing from left to right, and in each column – strictly increasing from top to bottom. Let $\pi \in \mathrm{Sym}_N$ be the unique permutation such that $A = \pi(A_\lambda)$ and put $e_A = \Pi_A e_\pi$. Then the vectors e_A, where A runs through all standard Young tableaux for the partition λ, form a basis of G_λ. In other words, the basis elements are obtained by successive symmetrization on the rows of Y_λ with a subsequent anti-symmetrization on the columns.

[03] Another choice of a Young tableau $A \in \mathfrak{T}_\lambda$ gives a Sym_N-module equivalent to G_λ.

The partition $\lambda = (N)$ corresponds to the Young diagram with only one row and produces the trivial representation of Sym_N. The partition $\lambda = (1, ..., 1)$ corresponds to the transposed Young diagram - a diagram with only one column - and produces another one-dimensional representation, the alternating representation $\pi \mapsto (-1)^{\varepsilon(\pi)}$. In general, let $\lambda' = (\lambda'_1, ..., \lambda'_m)$ be the partition conjugated to the partition λ, which is defined by transposing the Young diagram Y_λ by interchanging the rows and columns (λ'_i is the number of terms in the partition λ which are greater than or equal to i). Then

$$T_{\lambda'} = T_\lambda \otimes T_{(1,...,1)} \tag{3.6}$$

Other partitions correspond to the symmetries of mixed type.
The next result will play a crucial role in determining the symmetry properties of coordinate wave functions.

Proposition 3.2. The tensor product $T_\lambda \otimes T_\mu$ contains the trivial representation of Sym_N if and only if $\mu = \lambda$, in which case it has multiplicity one. In terms of a basis $\{e_i\}_{i=1}^{d_\lambda}$ in G_λ such that the representation T_λ is given by orthogonal $d_\lambda \times d_\lambda$ matrices $t_\lambda(\pi)_{ij}$,

$$T_\lambda(\pi)e_i = \sum_{j=1}^{d_\lambda} t_\lambda(\pi)_{ji} e_j, \quad i = 1, ..., d_\lambda$$

the one-dimensional subspace of the trivial representation is spanned by the vector $\sum_{i=1}^{d_\lambda} e_i \otimes e_i \in G_\lambda \otimes G_\lambda$. Correspondingly, the tensor product $T_\lambda \otimes T_\mu$ contains the alternating representation of Sym_N if and only if $\mu = \lambda'$, in which case it has multiplicity one. In terms of a basis $\{e'_i\}_{i=1}^{d_\lambda}$ in $G_{\lambda'}$ such that the representation $T_{\lambda'}$ is given by the matrices $t_{\lambda'}(\pi)_{ij} = (-1)^{\varepsilon(\pi)} t_\lambda(\pi)_{ij}$, the one-dimensional subspace of the alternating representation is spanned by the vector $\sum_{i=1}^{d_\lambda} e_i \otimes e'_i \in G_\lambda \otimes G_{\lambda'}$.
Problem 3.1. Prove all the statements in this section. (Hint: See the list of references to this chapter).
3.3. Schur-Weyl duality and symmetry of the wave functions. In addition to the diagonal action of the Lie group SU(2) in the tensor product $(\mathbb{C}^2)^{\otimes N}$, discussed in Section 3.1, there is also a left action of a symmetric group Sym_N by permuting factors [4]:

$$T(\pi)\,(v_1 \otimes \cdots \otimes v_N) = v_{\pi^{-1}(\mathbf{1})} \otimes \cdots \otimes v_{\pi^{-1}(N)}, \quad \pi \in \mathrm{Sym}_N$$

For every partition $\lambda \in \mathrm{Par}(N)$ denote by Π_λ the Young symmetrizer corresponding to the canonical Young tableau A_λ, and by $S_\lambda \mathbb{C}^2$ the image of the operator $T(\Pi_\lambda)$ in $(\mathbb{C}^2)^{\otimes N}$. The subspace $S_\lambda \mathbb{C}^2$ is zero-dimensional when the Young diagram Y_λ has more than two rows, and is an irreducible U(2)-module, called the Weyl module, when the Young diagram Y_λ has one or two rows. For the partition $\lambda = (N)$ the Weyl module $S_\lambda \mathbb{C}^2 = \mathrm{Sym}^N \mathbb{C}^2$ and is isomorphic to the highest weight module $V_{\lambda,N}$ with the dominant weight $(N, 0)$, defined in Section 1.2. For the partition $\lambda = (\lambda_1, \lambda_2)$ the Weyl module $S_\lambda \mathbb{C}^2$ is isomorphic to the highest weight module $V_{\lambda,N}$ with the dominant weight λ.

Remark. This construction is a special case of the general construction given by H . Weyl, which applies to the symmetric group action in the tensor product $V^{\otimes N}$, where V is a finite-dimensional vector space. The Weyl modules $S_\lambda V$ associated with the Young diagram Y_λ are zero-dimensional when the number of rows is greater than $n = \dim V$, and are isomorphic to the highest weight modules of $\mathrm{GL}(V)$ with the dominant weight λ when the number of rows is less than or equal to n. The association $V \mapsto S_\lambda V$ is called the Schur functor.

The following result, the Schur-Weyl duality, establishes explicit pairing between irreducible representations of U(2) and Sym_N that appear in the decomposition of the representation of $\mathrm{SU}(2) \times \mathrm{Sym}_N$ in $(\mathbb{C}^2)^{\otimes N}$ into the irreducible components.

Theorem 3.2 (Schur-Weyl duality). There is a direct sum decomposition into irreducible components of the representation $R_{\frac{1}{2}}^{\otimes N} \times T$:

$$\left(\mathbb{C}^2\right)^{\otimes N} = \bigoplus_{\lambda \in \mathrm{Par}(N,2)} S_\lambda \mathbb{C}^2 \otimes G_\lambda$$

where $\mathrm{Par}(N,2)$ is the set of partitions of N with number of terms less than or equal to 2 . Setting $\lambda_1 = \frac{N}{2} + s, \lambda_2 = \frac{N}{2} - s$ (cf. Section 1.2), from the Frobenius formula we obtain

$$d_\lambda = \dim G_\lambda = \binom{N}{\frac{N}{2} - s} - \binom{N}{\frac{N}{2} - s - 1}. \tag{3.7}$$

Now return to the main problem of finding total wave functions satisfying (3.5). It follows from the Schur-Weyl duality that there are $(2s+1)d_\lambda$ linear independent spin wave functions $\chi_{mj}(\sigma_1, ..., \sigma_N)$ of spin s satisfying

$$S^2 \chi_{mj} = s(s+1)\chi_{mj} \quad \text{and} \quad S_3 \chi_{mj} = m\chi_{mj} \tag{3.8}$$

where $m = -s, -s+1, ..., s-1, s$ and $j = 1, ..., d_\lambda$. Here d_λ corresponds to the partition $\lambda = \left(\frac{N}{2} + s, \frac{N}{2} - s\right)$ (or $\lambda = (N)$ for $s = \frac{N}{2}$) and is given by (3.7). The spin s representation ρ_s of $\mathrm{SU}(2)$ acts on the index m of the spin wave function $\chi_{mj}(\sigma_1, ..., \sigma_N)$, and the representation T_λ of Sym_N acts on the index j. The total wave function has the form

$$\Phi_m(\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_N) = \sum_{j=1}^{d_\lambda} \Psi_j(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)\, \chi_{mj}(\sigma_1, ..., \sigma_N) \tag{3.9}$$

where $m = -s, ..., s$. It follows from Proposition 3.2 that the total wave function $\Phi_m(\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_N)$ is totally anti-symmetric if and only if the coordinate wave functions $\Psi_j(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)$ transform according to the conjugated representation $T_{\lambda'}$ of Sym_N,

$$(P_\pi \Psi_i)(\boldsymbol{x}_1, ..., \boldsymbol{x}_N) = \sum_{j=1}^{d_\lambda} t_{\lambda'}(\pi)_{ji} \Psi_j(\boldsymbol{x}_1, ..., \boldsymbol{x}_N), \quad i = 1, ..., d_\lambda \tag{3.10}$$

We summarize these results as follows.

Theorem 3.3. Coordinate wave functions $\Psi_j(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)$ associated with the total wave function of spin s of a system of N identical particles of spin $\frac{1}{2}$ are those solutions of the N-particle Schrdinger equation (3.4) that transform according to the representation $T_{\lambda'}$ of the symmetric group Sym_N, where λ' is a conjugated partition to $\lambda = \left(\frac{N}{2} + s, \frac{N}{2} - s\right)$. The spin wave functions $\chi_{mj}(\sigma_1, ..., \sigma_N)$ satisfy (3.8), and corresponding total wave functions $\Phi_m(\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_N)$ are given by (3.9). In general, for a given energy level E there are $2s+1$ linearly independent total wave functions of spin s, $0 \le s \le \frac{N}{2}$, and $\frac{N}{2} - s$ is an integer.

Remark. For the highest value of total spin $s = \frac{N}{2}$ the coordinate wave function $\Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)$ is totally anti-symmetric. Since $(N)' = (1, ..., 1) \notin \mathrm{Par}(N,2)$ when $N > 2$, coordinate wave function for the case $N > 2$ is never totally symmetric.

Using explicit description of the Young symmetrizer in the previous section, we obtain the following result.

Corollary 3.4 (V.A. Fock). The coordinate wave function $\Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)$ associated with the total wave function of spin s is characterized by the following symmetry properties.

(i) $\Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)$ is anti-symmetric with respect to the group of arguments $\boldsymbol{x}_1, ..., \boldsymbol{x}_k, k = \frac{N}{2} + s$.

(ii) $\Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)$ is anti-symmetric with respect to the group of arguments $\boldsymbol{x}_{k+1}, ..., \boldsymbol{x}_N$.

(iii) $\Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N)$ satisfies

[04] It moves the vector in the i-th place of the tensor product to the $\pi(i)$-th place.

$\Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N) = \sum_{i=1}^{k} \Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_{i-1}, \boldsymbol{x}_{k+1}, \boldsymbol{x}_{i+1}, ..., \boldsymbol{x}_k, \boldsymbol{x}_i, \boldsymbol{x}_{k+2}, ..., \boldsymbol{x}_N)$.
The case of N identical particles of arbitrary spin s is treated similarly. The symmetry properties of coordinate wave functions can be obtained by using Schur-Weyl duality for the action of $\mathrm{U}(l) \times \mathrm{Sym}_N$ in $\mathbb{C}^l$, where $l = 2s + 1$. It has the form

$$\left(\mathbb{C}^l\right)^{\otimes N} = \bigoplus_{\lambda \in \mathrm{Par}(N,l)} S_\lambda \mathbb{C}^l \otimes G_\lambda,$$

where $\mathrm{Par}(N, l)$ is the set of partitions of N with number of terms less than or equal to l, and $S_\lambda \mathbb{C}^l$ is the Weyl module corresponding to the highest weight representation of $\mathrm{U}(l)$ with the dominant weight λ.

Problem 3.2. Prove Corollary 3.4.

Problem 3.3 (One-electron approximation). Suppose that $V_{\text{int}}(\boldsymbol{x}) = 0$, and let $\psi_1(\boldsymbol{x}), ..., \psi_k(\boldsymbol{x}), k \geq \frac{N}{2}$, be the one-electron wave functions: eigenfunctions of the one-electron Schrdinger operator H_1 (see (3.4)). Show that the coordinate wave function

$$\Psi(\boldsymbol{x}_1, ..., \boldsymbol{x}_N) = \begin{vmatrix} \psi_1(\boldsymbol{x}_1) & ... & \psi_1(\boldsymbol{x}_k) \\ ... & ... & ... \\ \psi_k(\boldsymbol{x}_1) & ... & \psi_k(\boldsymbol{x}_k) \end{vmatrix} \begin{vmatrix} \psi_1(\boldsymbol{x}_{k+1}) & ... & \psi_1(\boldsymbol{x}_N) \\ ... & ... & ... \\ \psi_{N-k}(\boldsymbol{x}_{k+1}) & ... & \psi_{N-k}(\boldsymbol{x}_N) \end{vmatrix},$$

where $|\cdots|$ stands for the matrix determinant, satisfy the symmetry properties in Corollary 3.4.

5 Other Fundamental Questions of Quantum Mechanics

5.1 Established Ideas of Generalizations of Quantum Mechanics

5.1.1 Idea of Relativistic QM

(intro to rel QM, not focused on models, since they are in the next part)

5.1.2 Idea of QFT

(intro to this generalization of QM, see special note about it)

5.2 Other About the Fundamentals of Quantum Mechanics

5.2.1 General Philosophical Features of QM

Почему у частиц одни параметры квантуются (принимают разные значения с разной вероятностью), а другие нет?

Например, закон взаимодействия - один и тот же, потенциалы - для моделей - одни и те же, а координата и импульсы - да самые разные с плотностью вероятности, которая подчиняется уравнению Шредингера.

почему именно так?

почему другие параметры тоже не принимали бы разные значения с разной вероятностью?

что если заряд бы тоже был разный?

или потенциал разный? (причем не от беспорядка, а от просто какой-то квантовости природы потенциала)

5.2.2 Coulomb Interaction in scope of QM in Details

(discuss how exactly a particle is throwing a virtual photon to another one. this is written in QFT now. See Zi's book about it. a big big question!!!)

5.2.3 Examples of the Inconsistency of Quantum Mechanics

(Севрин там пару привел, тут потом напишу их)

Ненулевая вероятность частицы появиться вне светового конуса

(пропишу этот вывод)

Отрицательная норма действия оператора рождения (???)

(пропишу этот вывод, Севрин на лекции сказал, не так это и важно, но интересно.)

5.2.4 Bell Inequality (!!?)

Обсудим подробно неравенство Белла
(популярно про него из первой части, ибо часто про это поговорить хочется. тут многое можно сказать)

Вывод

Пример применения

О популярных интерпретациях

Как догадаться про это?

5.2.5 Experimental Verification of the Bell Inequality (!!?)

(!! тут Нобелевская премия за это!!)
(см. Experimental Realization of Einstein-Podolsky-Rosen-Bohm Gedankenexperiment: A New Violation of Bell's Inequalities Alain Aspect, Philippe Grangier, and Gdrard Roger. пока все равно не разбираюсь в этом, пока хз.)

5.2.6 On the Directions of Possible Generalizations of Quantum Mechanics

(это раздел про основы, так что тоже укажем, что вообще как можно было бы модифицировать. конкретно модификации - или в конце записи или в отдельной папке с теорфизическими теориями)

5.2.7 On Misunderstandings of Quantum Mechanics by Physicists in General

Часто можно встретить людей, не понимающих, что такое квантовая механика. Таким людям правильнее уволится и вообще не заниматься физикой. А я помню заблуждения в типичных шаблонах их рассказов.
(напишу потом их, потом мб сделаю большой список, но рыться в этом вообще не актуально, лучше другими делами 100 другими делами заниматься, чем думать про неверные понимания)

Об заблуждении про электронное облако

Об заблуждении про существование размеров элементарной частицы

5.3 Other Fundamental Properties of Quantum Systems

5.3.1 Entropy of a Quantum System

5.3.2 Connection of Entropy and Geometry

(?? I'll lean it someday later, maybe)

5.3.3 Kramers Theorem on Time Reversal(???)

Суть

In quantum mechanics, the Kramers' degeneracy theorem states that for every energy eigenstate of a time-reversal symmetric system with halfinteger total spin, there is another eigenstate with the same energy related by time-reversal. In other words, the degeneracy of every energy level is an even number if it has half-integer spin. The theorem is named after Dutch physicist H. A. Kramers. In theoretical physics, the time reversal symmetry is the symmetry of physical laws under a time reversal transformation:

$$T : t \mapsto -t$$

If the Hamiltonian operator commutes with the time-reversal operator, that is

$$[H, T] = 0$$

then, for every energy eigenstate $|n\rangle$, the time reversed state $T|n\rangle$ is also an eigenstate with the same energy. These two states are sometimes called a Kramers pair [1] In general, this time-reversed state may be identical to the original one, but that is not possible in a half-integer spin system: since time reversal reverses all angular momenta, reversing a half-integer spin cannot yield the same state (the magnetic quantum number is never zero).

Обзор применений (???)

(слышал, но не знаю, зачем она)

5.3.4 Time-Reversal Symmetry: Advanced Features

(people are really fascinating with this topic, I don't know why, but I am assured that there are a lot of things to write about it)

Part III
Typical Methods and Models

6 Main General Methods and Templates

6.1 Overview of Different Method for Solving Problems in QM

(general ideas about what can be done and when it is a good idea to use this method?)

PT

Adiabatics

Averaging (extra integration)

(???? discuss how good this method is??? a problem about anisotropic spectrum is solved by it)

6.2 Perturbation Theory: Fundamentals

Обсудим подробно теорию возмущений.

6.2.1 RS Stationary Perturbation Theory, Non-Degenerate Case

Обсудим подробно стационарную теорию возмущений. By "RS" I mean Rayleigh-Schrodinger, since there are also other perturbation theories.

Стационарная теория возмущений в невырожденном случае

Вывод формул

Пусть известны точные решения стационарного уравнения с гамильтонианом $\hat{H}_0$:

$$\hat{H}_0 \left|n^{(0)}\right\rangle = E_n^{(0)} \left|n^{(0)}\right\rangle,$$

где $\left|n^{(0)}\right\rangle$ - невырожденные состояния дискретного спектра с энергией $E_n^{(0)}$. Рассмотрим спектральную задачу с гамильтонианом

$$\hat{H} = \hat{H}_0 + \lambda V, \quad \lambda \to 0,$$

где возмущение V не зависит от времени, так же как и исходный гамильтониан $\hat{H}_0$. В силу предельного перехода $\lambda \to 0$ будем полагать, что базис гильбертова пространства $\left|n^{(0)}\right\rangle$ полон и в гильбертовом пространстве и в задаче с возмущением. Это предположение является центральным в теории возмущений! Если оно a posteriori оказывается неверным, то теория возмущений теряет всякий смысл. (????? why?????)

Нас будет интересовать только дискретный спектр в задаче с возмущением, так как в силу центрального предположения применимости теории возмущений, области непрерывного спектра в задаче с возмущением и без него совпадают, а дискретные же уровни энергии могут смещаться. (????? why?????)

Будем искать собственные значения

$$\hat{H}|n\rangle = E_n|n\rangle$$

в виде ряда по $\lambda \to 0$:

$$E_n = E_n^{(0)} + \sum_{p=1}^{\infty} \lambda^p \epsilon_p,$$

где ϵ_p-поправка p-го порядка. Собственные векторы состояний также можно записать в виде ряда

$$|n\rangle = \left|n^{(0)}\right\rangle + \sum_{p=1}^{\infty} \lambda^p \left|n^{(p)}\right\rangle.$$

Однако собственные состояния гамильтониана допускают несингулярное преобразование

$$|n\rangle \mapsto f(\lambda)|n\rangle, \quad f(0) = 1.$$

Поэтому для того, чтобы разложение состояния в ряд по λ было однозначным, необходимо зафиксировать амплитуду вероятности одного из базисных векторов исходного гильбертова пространства, например, $\left|n^{(0)}\right\rangle$. (????? why?????)

Here, we will be building our PT with by using the condition

$$\left\langle n^{(0)}|n\right\rangle = 1.$$

This is not the only way. One can take another condition (??? did I wrote it below???).

Подставляя сюда $|n\rangle = \left|n^{(0)}\right\rangle + \sum\limits_{p=1}^{\infty} \lambda^p \left|n^{(p)}\right\rangle$ и рассматривая его последовательно в каждом порядке, находим, что

$$\left\langle n^{(0)}|n^{(p)}\right\rangle = 0,$$

т. е. каждая поправка к состоянию не содержит вклада $\left|n^{(0)}\right\rangle$ и, следовательно, ортогональна исходному невозмущенному состоянию. Note, that here n is the selected level, in which we are interested. We don't consider here other levels at all.

Конечно, выбор условия однозначности в форме (15.6) приводит к собственному вектору, норма которого, вообще говоря, отлична от единицы, но эта проблема легко решается последовательно в любом заданном наперед порядке по λ. (??? how exactly??)

Подставляя разложения в $\hat{H}|n\rangle = E_n|n\rangle$, находим

$$\left(\hat{H}_0 + \lambda V\right)\left\{\left|n^{(0)}\right\rangle + \sum_{p=1}^{\infty} \lambda^p \left|n^{(p)}\right\rangle\right\} = \left(E_n^{(0)} + \sum_{p=1}^{\infty} \lambda^p \epsilon_p\right)\left\{\left|n^{(0)}\right\rangle + \sum_{p=1}^{\infty} \lambda^p \left|n^{(p)}\right\rangle\right\},$$

так что последовательно в каждом порядке по λ получаем рекуррентную систему уравнений:

$$\begin{aligned}
&\lambda^0 : \hat{H}_0 \left|n^{(0)}\right\rangle = E_n^{(0)} \left|n^{(0)}\right\rangle, \\
&\lambda^1 : \hat{H}_0 \left|n^{(1)}\right\rangle + V \left|n^{(0)}\right\rangle = E_n^{(0)} \left|n^{(1)}\right\rangle + \epsilon_1 \left|n^{(0)}\right\rangle, \\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
&\lambda^p : \hat{H}_0 \left|n^{(p)}\right\rangle + V \left|n^{(p-1)}\right\rangle = E_n^{(0)} \left|n^{(p)}\right\rangle + \epsilon_1 \left|n^{(p-1)}\right\rangle + \ldots + \epsilon_p \left|n^{(0)}\right\rangle.
\end{aligned}$$

Пользуясь ортогональностью поправок и состояния $\left|n^{(0)}\right\rangle$ и исходным уравнением $\left\langle n^{(0)}\right| \hat{H}_0 = \left\langle n^{(0)}\right| E_n^{(0)}$, возьмем проекцию уравнений выше на это состояние: $\left\langle n^{(0)}|\cdot\right\rangle$, так что

$$\begin{aligned}
&\epsilon_1 = \left\langle n^{(0)}|V|n^{(0)}\right\rangle = V_{nn},\\
&\epsilon_2 = \left\langle n^{(0)}|V|n^{(1)}\right\rangle,\\
&\ldots\ldots\ldots\ldots\ldots\ldots\\
&\epsilon_p = \left\langle n^{(0)}|V|n^{(p-1)}\right\rangle,
\end{aligned}$$

т. е. опять-таки рекуррентную схему вычисления поправок к энергии, если известны поправки к состоянию.

Поправки к состоянию в силу их ортогональности к уровню $\left|n^{(0)}\right\rangle$ в базисе исходной задачи раскладываются в виде

$$\left|n^{(p)}\right\rangle = \sum_{k\neq n} \left|k^{(0)}\right\rangle \left\langle k^{(0)}|n^{(p)}\right\rangle,$$

(?? not fully sure, why here $k \neq n$?? of course, if $k = n$, then we will have $|n^{(0)}\rangle$, which is not in order we want, but is there a derivation of this formula??) At this point, we start working with not only the needed state $\left|n^{(0)}\right\rangle$, but with any other.

Амплитуды разложения легко найти, проецируя уравнения

$$\begin{aligned}
&\lambda^0 : \hat{H}_0 \left|n^{(0)}\right\rangle = E_n^{(0)} \left|n^{(0)}\right\rangle,\\
&\lambda^1 : \hat{H}_0 \left|n^{(1)}\right\rangle + V \left|n^{(0)}\right\rangle = E_n^{(0)} \left|n^{(1)}\right\rangle + \epsilon_1 \left|n^{(0)}\right\rangle,\\
&\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\\
&\lambda^p : \hat{H}_0 \left|n^{(p)}\right\rangle + V \left|n^{(p-1)}\right\rangle = E_n^{(0)} \left|n^{(p)}\right\rangle + \epsilon_1 \left|n^{(p-1)}\right\rangle + \ldots + \epsilon_p \left|n^{(0)}\right\rangle.
\end{aligned}$$

на состояния базиса $\left\langle k^{(0)}|\cdot\right\rangle$:

$$\begin{aligned}
\left\langle k^{(0)}|V|n^{(0)}\right\rangle &= \left(E_n^{(0)} - E_k^{(0)}\right) \left\langle k^{(0)}|n^{(1)}\right\rangle,\\
\left\langle k^{(0)}|V|n^{(p-1)}\right\rangle &= \left(E_n^{(0)} - E_k^{(0)}\right) \left\langle k^{(0)}|n^{(p)}\right\rangle + \epsilon_1 \left\langle k^{(0)}|n^{(p-1)}\right\rangle + \ldots + \epsilon_{p-1} \left\langle k^{(0)}|n^{(1)}\right\rangle.
\end{aligned}$$

Now, we plug out term $\left\langle k^{(0)}|n^{(p)}\right\rangle$ after term for increasing p, and we see that for p-th term, the general formula holds:

$$\left\langle k^{(0)}|n^{(p)}\right\rangle = \frac{1}{E_n^{(0)} - E_k^{(0)}} \left\{ V_{kn}^{(p-1)} - \epsilon_1 \left\langle k^{(0)}|n^{(p-1)}\right\rangle - \ldots - \epsilon_{p-1} \left\langle k^{(0)}|n^{(1)}\right\rangle \right\},$$

где $p \geqslant 1, k \neq n,\ V_{kn}^{(p-1)} := \left\langle k^{(0)}|V|n^{(p-1)}\right\rangle$.

So, we got formula for $\left\langle k^{(0)}|n^{(p)}\right\rangle$, which will be immediately used in calculation of energy shift by $\epsilon_p = \left\langle n^{(0)}|V|n^{(p-1)}\right\rangle$.

In particular,

$$\left|n^{(1)}\right\rangle = \sum_{k\neq n} \frac{V_{kn}}{E_n^{(0)} - E_k^{(0)}} \left|k^{(0)}\right\rangle,$$

откуда

$$\epsilon_2 = \sum_{k\neq n} \frac{V_{nk} V_{kn}}{E_n^{(0)} - E_k^{(0)}},$$

и в силу $V_{nk} = \langle n^{(0)}|V|k^{(0)}\rangle = \langle k^{(0)}|V|n^{(0)}\rangle^* = V_{kn}^*$,

$$\epsilon_2 = \sum_{k\neq n} \frac{|V_{kn}|^2}{E_n^{(0)} - E_k^{(0)}}.$$

Отсюда, в частности, следует, что для основного состояния с наименьшей энергией $E_n^{(0)} - E_k^{(0)} < 0$ поправка второго порядка всегда отрицательна, если не равна нулю.

Подчеркнем, что ведущая поправка к энергии уровня задается средним значением возмущения. По смыслу теории возмущений поправки высших порядков становятся существенны, если поправки низшего порядка обращаются в нуль или необходимо получить значение с высокой точностью.

Условия применимости стационарной теории возмущений

(укажу то, что вначале Киселев писал.)

Необходимым условием применимости теории возмущений является сходимость рядов для энергий и собственных состояний системы с $\hat{H} = \hat{H}_0 + \lambda V$. Мы установили, что поправки к состояниям строятся по степеням малого отношения матричного элемента возмущения к инкременту уровней в исходной системе

$$\frac{|V_{kn}|}{\Delta E_{kn}^{(0)}} \ll 1.$$

Значит, возмущение можно считать малым, если его характерная величина, т. е. модуль его матричных элементов между векторами стационарных состояний невозмущенной задачи, отвечающими различным уровням энергии, существенно меньше типичного расстояния между этими уровнями. С физической точки зрения это означает, что возмущение не приводит к «перекрытию уровней исходной системы. В этом случае вклад высших поправок к состояниям подавлен степенями этого малого параметра, так что из выражения для поправок к энергии (15.9) следует, что и они также подавлены в зависимости от порядка p теории возмущений.

О случаях применения стационарной теории возмущений в невырожденном случае

Of course, mathematically - when we have a non-degenerate system, where there is no dynamics, just a complicated Hamiltonian. But when does it happens most often physically?

(?I'll write later)

О случаях неполного базиса, когда теория возмущений неприменима (???)

(Киселев сказал, что тогда смысла в ней нет, я пока что не понимаю, почему и когда такое может быть???)

Suppose we have system with two small perturbative terms. Поправки любых порядков от двух малых возмущений равны сумме поправок от каждого возмущения поотдельности

We always believe that this is so. But I want to also prove it.

(??? I haven't proven it yet, I don't have time to it and I am not sure, if there will be some problems with it.)

Особенности стационарной теории возмущений для типичных задач

(тут указания про задачи.)

О стационарной теории возмущений для осциллятора

(!!!! про операторы рождения и уничтожения написать нормально, пока слабая про них теория, а тут они очень нужны!!! особенно их преобразования!)

(!!! тут заготовки преобразований операторов рождения и уничтожения, типичная ситуация, что приходится они них полиномы брать!)

(!! важно не переставлять лихо N и a a крест, потому что за счет них N становится другой!!! это приводит к ошибкам, напишу там про это.)

О стационарной теории возмущений для бесконечно глубокой потенциальной ямы

О стационарной теории возмущений для конечной потенциальной ямы (!?!??!!??!?!?)

(вот тут прямо я хз, как делать, опыта нет.)

О стационарной теории возмущений для возмущения вида дельта-потенциала (!?!??!!??!?!?)

(вот тут прямо я хз, как делать, опыта нет. она вообще применима для этого случая?)

Математические указания для работы с теорией возмущений (!?!?)

(это важно, без этого ничего не сделаешь, упершись только в математику.)

Как догадаться про RS PT?

(??? left question)

6.2.2 RS Stationary Perturbation Theory, Degenerate Case

Стационарная теория возмущений в вырожденном случае

(с этим пока что не освоился.)

Вывод формул

Если уровень исходной системы $E_n^{(0)}$ является вырожденным и кратность его вырождения равна k, то предел $\lambda \to 0$ в системе с возмущением также можно определить однозначно, фиксировав вклад ортонормированных базисных собственных векторов в k-мерном подпространстве с энергией $E_n^{(0)}$

$$\hat{H}_0 \left|n^{(0)}, a\right\rangle = E^{(0)} \left|n^{(0)}, a\right\rangle, \quad a \in \{\overline{1,k}\}, \quad \left\langle n^{(0)}, b | n^{(0)}, a\right\rangle = \delta_{ab},$$

в состояние

$$|n\rangle = \sum_{a=1}^{k} C_a \left|n^{(0)}, a\right\rangle + \sum_{p=1}^{\infty} \lambda^p \left|n^{(p)}\right\rangle,$$

т. е. задав «вектор» $C_a = \langle n^{(0)}, a|n\rangle$.

Отсюда опять следует, что поправки по построению ортогональны подпространству состояний с энергией $E_n^{(0)}$.

Используя разложение в ряд энергии и состояния, в полной аналогии с невырожденным случаем в первом порядке по λ находим

$$\hat{H}_0 \left|n^{(1)}\right\rangle + V \sum_{a=1}^{k} C_a \left|n^{(0)}, a\right\rangle = E_n^{(0)} \left|n^{(1)}\right\rangle + \epsilon_1 \sum_{a=1}^{k} C_a \left|n^{(0)}, a\right\rangle .$$

Проецируя это уравнение на $\langle n^{(0)}, b|\cdot\rangle$ с учетом уравнения на собственные значения гамильтониана $\hat{H}_0$ и ортогональности поправок ведущему вкладу за счет $\left|n^{(0)}, b\right\rangle$, получаем уравнение

$$\sum_{a=1}^{k} \{V_{ba} - \epsilon_1 \delta_{ba}\} C_a = 0, \quad V_{ba} = \langle n^{(0)}, b|V|n^{(0)}, a\rangle ,$$

которое говорит о том, что вектор C_a является собственным для эрмитовой матрицы V_{ab}, и его собственное значение ϵ_1 дает величину ведущей поправки к энергии этого состояния. Секулярное уравнение для матрицы $\|\hat{V}\|_{ba} = V_{ba}$ в подпространстве собственных состояний энергии $E_n^{(0)}$

$$\det(\hat{V} - \epsilon) = 0$$

имеет k собственных значений, которые, вообще говоря, тоже могут быть вырождены. Выбирая значения C_a в виде собственных векторов матрицы $\hat{V}$, находим «правильные» функции ведущего приближения

$$\left|\tilde{n}^{(0)}, g\right\rangle , \quad \hat{V} \left|\tilde{n}^{(0)}, g\right\rangle = \epsilon_1^{(g)} \left|\tilde{n}^{(0)}, g\right\rangle ,$$

где g нумерует собственные значения матрицы $\hat{V}$. Поскольку правильные функции составляют ортогональный базис, задача нахождения высших поправок теперь сводится к решению тех же рекуррентных соотношений, что и в невырожденном случае, для каждого из собственных векторов матрицы $\hat{V}$:

$$\hat{H}_0 \left|n^{(p)}\right\rangle + V \left|n^{(p-1)}\right\rangle = E_n^{(0)} \left|n^{(p)}\right\rangle + \epsilon_1^{(g)} \left|n^{(p-1)}\right\rangle + ... + \epsilon_p^{(g)} \left|n^{(0)}, g\right\rangle .$$

Дальнейшее построение повторяет рассмотрение невырожденного случая. При этом поправки к состояниям могут включать в себя и вырожденные состояния уровней энергии исходного гамильтониана, отличных от рассматриваемого уровня $E_n^{(0)}$.

О случаях применения стационарной теории возмущений в вырожденном случае (???)

Важно понимать, какие модели могут иметь вырождение, чтобы потом оно снималось возмущением.

(?? и какие же??)

В более чем 1-мерном осцилляторе, оказывается, применяется.

Второй порядок вырожденной теории возмущений

Разумеется, может быть ситуация, в которой возмущение не снимается в первом порядке (или снимается лишь частично) - в таком случае нужно двигаться дальше. Опять-таки, мы используем уравнение (5.3):

$$\hat{H}_0 \left|n^{(2)}\right\rangle + \hat{V} \left|n^{(1)}\right\rangle = E_n^{(2)} \left|n^{(0)}\right\rangle + E_n^{(1)} \left|n^{(1)}\right\rangle + E_n^{(0)} \left|n^{(2)}\right\rangle$$

Тут мы ограничимся лишь поправкой второго порядка к уровням энергии, поэтому спроецируем сразу это уравнение на $\left\langle n_\alpha^{(0)}\right|$:

$$\sum_{m\neq n,\beta}\frac{V_{\alpha m}V_{m\beta}}{\omega_{nm}}c_{n,\beta}^{(0)}\equiv\sum_{\beta}H_{\alpha\beta}^{(\text{eff})}c_{n,\beta}^{(0)}=E_n^{(2)}c_{n,\alpha}^{(0)},\quad H_{\alpha\beta}^{(\text{eff})}=\sum_{m\neq n}\frac{V_{\alpha m}V_{m\beta}}{\omega_{nm}}$$

Полученное уравнение, как и в первом порядке, устроено в точности как уравнение Шрёдингера, спроецированное на вырожденное подпространство, но с эффективным гамильтонианом $H^{(\text{eff})}$ (который раньше попросту совпадал с $\hat{V}$). Поступать с ним нужно точно так же - если вырождение не было снято в первом порядке, то поправки второго порядка определяются секулярным уравнением $\det\left(\hat{H}^{(\text{eff})}-E_n^{(2)}\right)=0$, а правильные волновые функции ведущего приближения будут соответствовать этим уровням энергии.

Про эффективный гамильтониан можно думать, как про вклад виртуальных переходов с одного из уровней вырожденного подпространства $E_\alpha^{(0)}$ на невырожденный уровень $E_m^{(0)}$ и обратно на уровень $E_\beta^{(0)}$, принадлежащий тому же вырожденному подпространству $\left(E_\alpha^{(0)}=E_\beta^{(0)}\right)$, но не обязательно являющийся тем же состоянием (только для $\alpha=\beta$).

О случаях применения стационарной теории возмущений в вырожденном случае во втором порядке (???)

(вообще хз, ни разу не применял, но по идее могло бы такое понадобиться.)

Задача с двумя уровнями

Рассмотрим задачу с только два уровнями с гамильтонианом $\hat{H}_0+\lambda V$. Решение представляется в виде разложения

$$|\psi\rangle=c_1|1\rangle+c_2|2\rangle,$$

где эти состояния такие, что $\hat{H}_0|1\rangle=E_1^{(0)}|1\rangle$, $\hat{H}_0|2\rangle=E_2^{(0)}|2\rangle$. Подставим в уравнение $\hat{H}|\psi\rangle=E|\psi\rangle$, получим:

$$H_{11}c_1+\lambda V_{12}c_2=Ec_1$$
$$H_{22}c_2+\lambda V_{21}c_1=Ec_2$$

или в матричном виде

$$\begin{pmatrix}H_{11}&\lambda V_{12}\\ \lambda V_{12}^*&H_{22}\end{pmatrix}\begin{pmatrix}c_1\\c_2\end{pmatrix}=E\begin{pmatrix}c_1\\c_2\end{pmatrix},$$

т. е. уравнение на собственные значения матрицы 2×2.

(??? тут можно лучше написать. Судя по всему, возмущение кросдиагональное предполагается, окей. потом напишу лучше.)

Решаем:

$$\det\{\hat{H}-E\}=\left[\frac{1}{2}\left(H_{11}+H_{22}\right)-E\right]^2-\frac{1}{4}\left(H_{11}-H_{22}\right)^2-\lambda^2\left|V_{12}\right|^2=0.$$

Решения этого уравнения

$$E_\pm=\frac{1}{2}\left(H_{11}+H_{22}\right)\pm\sqrt{\frac{1}{4}\left(H_{11}-H_{22}\right)^2+\lambda^2\left|V_{12}\right|^2}$$

суть искомые значения энергии стационарных состояний, а соответствующие состояния в исходном базисе удобно выразить в виде унитарного поворота

$$|\psi_+\rangle = \mathrm{e}^{\mathrm{i}\phi/2}\sin\frac{\alpha}{2}|1\rangle + \mathrm{e}^{-\mathrm{i}\phi/2}\cos\frac{\alpha}{2}|2\rangle,$$
$$|\psi_-\rangle = \mathrm{e}^{\mathrm{i}\phi/2}\cos\frac{\alpha}{2}|1\rangle - \mathrm{e}^{-\mathrm{i}\phi/2}\sin\frac{\alpha}{2}|2\rangle$$

где мы ввели фазу ϕ матричного элемента $V_{12} = |V_{12}|\,\mathrm{e}^{\mathrm{i}\,\phi}$ и угол поворота α, так что

$$\operatorname{tg}\frac{\alpha}{2} = -\frac{\lambda\,|V_{12}|}{\frac{1}{2}\,(H_{11}-H_{22}) - \sqrt{\frac{1}{4}\,(H_{11}-H_{22})^2 + \lambda^2\,|V_{12}|^2}},$$

откуда

$$\operatorname{tg}\alpha = -\frac{2\lambda\,|V_{12}|}{H_{11}-H_{22}}.$$

В эти выражения входят значения диагональных матричных элементов гамильтониана

$$H_{11} = E_1^{(0)} + \lambda V_{11}, \quad H_{22} = E_2^{(0)} + \lambda V_{22},$$

которые при $E_1^{(0)} \neq E_2^{(0)}$ получались бы в стационарной теории возмущений в ведущем порядке по $\lambda \to 0$ без учета смешивания исходных состояний, в случае, когда точное решение (15.27) можно разложить до второго порядка по малому отношению

$$\left|\frac{\lambda V_{12}}{H_{11}-H_{22}}\right| \ll 1$$

При достаточно большой константе связи возмущения λ поведение собственных значений гамильтониана $E_\pm$, описываемое (15.27), будет качественно отличаться от поведения ведущего приближения в (15.30). Например, при некоторых фиксированных $E_1^{(0)} \neq E_2^{(0)}, V_{11} > 0, V_{22} < 0$ и $V_{12} \neq 0$ зависимость от λ для диагональных элементов гамильтониана и его собственных значений проиллюстрирована на рис. 26.

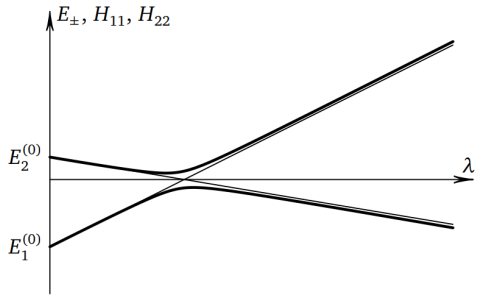


Figure 6.1: Зависимость собственных значений гамильтониана $E_\pm$(жирные линии) и диагональных элементов H_{11}, H_{22} (тонкие линии) от константы связи возмущения λ

Как видим, возмущение может быть настолько сильным, что в ведущем приближении диагональные матричные элементы имеют точку пересечения. Однако точное решение показывает, что истинные значения собственных значений гамильтониана не пересекаются. Поскольку допустимая область изменения угла $\alpha \in [0, \pi]$, собственные состояния гамильтониана являются смешанными за исключением исходной задачи с $\lambda = 0$ и при $\alpha \to \pi$, если $|V_{12}| \ll |V_{11} - V_{22}|$ и $\lambda \to \infty$, когда состояния $|1\rangle$ и $|2\rangle$ меняются местами: первое имеет большую энергию, чем второе.

Задача с двумя уровнями находит применение не только в случае, например, двух спиновых состояний для частицы со спином 1/2, но и в таких ситуациях, когда энергетическая щель между парой низших уровней энергии и их возбуждениями достаточно велика, чтобы можно было пренебречь вкладами от высших поправок от возбужденных состояний, в то время как эффекты смешивания за счет введения V велики и не могут быть рассмотрены как малые поправки в системе двух низших состояний.

О применениях (!??!)

(мб их много, укажу там потом.)

О случае, если два уровня вырождены (??)

(?? мы же решали только для одного вырожденного уровня, да? или все норм, просто то, на котором мы находились, расщепляется и все? а другие не будут расщепляться??? наверное, нет, все не норм.)

Математические указания для работы с (!?!?)

(это важно, без этого ничего не сделаешь, упершись только в математику.)

О деталях (!????!?!?!)

(тут вопросы, на которые пока я не нашел ответ. ну и не так важно.)

теория возмущений для перехода в основное состояние (??)

. Вообще у нас энергия уходит в фотон ведь? То есть это же теория излучения??? . В общем, как считать такие переходы??? Если волновая функция в основном - ноль, так что туда вообще не может перейти частица. .

теория возмущений при переходе к вырожденному уровню энергии (??)

Например, в осцилляторе переходы между ненулевыми уровнями.

Переход вырожденного случая в невырожденный случай (?!?!??!)

(остался вопрос, как этот преход происходит??? там же не супер мгновенно, а хотя бы какая-то плавность расщепления уровней должна быть??? пока не могу вывести эту плавность, одна и вторая теория есть, все, больше ничего. потом опишу этот переход.)

6.2.3 Brillouin-Wigner Perturbation Theory

Overview and derivation

(here are two pages by K. Ingersent)

Brillouin-Wigner (BW) perturbation theory is less widely used than the Rayleigh-Schrödinger (RS) version. At first order in the perturbation, the two theories are equivalent. However, BW perturbation theory extends more easily to higher orders, and avoids the need for separate treatment of non-degenerate and degenerate levels.

- Assume that we know the stationary states of the unperturbed Hamiltonian H_0, namely the kets $|n\rangle$ satisfying $H_0|n\rangle = \varepsilon_n|n\rangle$. For each unperturbed state, we can define a projection operator

$$Q_n = I - |n\rangle\langle n| = \sum_{m\neq n} |m\rangle\langle m|$$

Using the spectral representation $H_0 = \sum_n \varepsilon_n|n\rangle\langle n|$, one can see that $[H_0, Q_n] = 0$.

- Let us write the perturbed eigenproblem in the form

$$(E_n - H_0)\,|\psi_n\rangle = H_1\,|\psi_n\rangle\,.$$

Acting with Q_n from the left, and taking advantage of $[H_0, Q_n] = 0$,

$$Q_n\,|\psi_n\rangle = R_n H_1\,|\psi_n\rangle$$

where

$$R_n = (E_n - H_0)^{-1}\,Q_n = Q_n\,(E_n - H_0)^{-1}$$

which has a spectral representation

$$R_n = \sum_{m\neq n} \frac{|m\rangle\langle m|}{E_n - \varepsilon_m}$$

Note that R_n is not a projection operator because $R_n^2 \neq R_n$.

- Adopting the usual convention $\langle n \mid \psi_n\rangle = 1$, we can write

$$|\psi_n\rangle = |n\rangle + Q_n\,|\psi_n\rangle = |n\rangle + R_n H_1\,|\psi_n\rangle\,.$$

Assuming that H_1 is small, this equation can be solved iteratively in powers of H_1. The wave function correct through order j, $\left|\psi_n^{(j)}\right\rangle$, can be obtained from Eq. (2) by inserting $\left|\psi_n^{(j-1)}\right\rangle$ on the right-hand side:

$$\begin{aligned}
\left|\psi_n^{(0)}\right\rangle &= |n\rangle \\
\left|\psi_n^{(1)}\right\rangle &= |n\rangle + R_n H_1|n\rangle \\
\left|\psi_n^{(2)}\right\rangle &= |n\rangle + R_n H_1|n\rangle + (R_n H_1)^2\,|n\rangle \\
&\quad \text{etc}
\end{aligned}$$

In other words,

$$|\psi_n\rangle = \sum_{j=0}^{\infty} (R_n H_1)^j\,|n\rangle \equiv (1 - R_n H_1)^{-1}\,|n\rangle$$

where the first equality serves to define $(1 - R_n H_1)^{-1}$. Substituting the spectral representation of R_n into Eq. (3), we obtain

$$\begin{aligned}|\psi_n\rangle =& |n\rangle + \sum_{m\neq n} |m\rangle \frac{\langle m|H_1|n\rangle}{E_n - \varepsilon_m} + \sum_{m\neq n}\sum_{l\neq n} |m\rangle \frac{\langle m|H_1|l\rangle\langle l|H_1|n\rangle}{(E_n - \varepsilon_m)(E_n - \varepsilon_l)} \\ &+ \sum_{m\neq n}\sum_{l\neq n}\sum_{k\neq n} |m\rangle \frac{\langle m|H_1|l\rangle\langle l|H_1|k\rangle\langle k|H_1|n\rangle}{(E_n - \varepsilon_m)(E_n - \varepsilon_l)(E_n - \varepsilon_k)} + \ldots\end{aligned}$$

- We can obtain E_n by applying $\langle n|$ to Eq. (1):

$$(E_n - \varepsilon_n)\langle n \mid \psi_n\rangle = \langle n|H_1|\psi_n\rangle$$

Since $\langle n \mid \psi_n\rangle = 1$,

$$E_n = \varepsilon_n + \langle n|H_1|\psi_n\rangle$$

or, making use of Eq. (4),

$$\begin{aligned}E_n =& \varepsilon_n + \langle n|H_1|n\rangle + \sum_{m\neq n} \frac{\langle n|H_1|m\rangle\langle m|H_1|n\rangle}{E_n - \varepsilon_m} \\ &+ \sum_{m\neq n}\sum_{l\neq n} \frac{\langle n|H_1|m\rangle\langle m|H_1|l\rangle\langle l|H_1|n\rangle}{(E_n - \varepsilon_m)(E_n - \varepsilon_l)} \\ &+ \sum_{m\neq n}\sum_{l\neq n}\sum_{k\neq n} \frac{\langle n|H_1|m\rangle\langle m|H_1|l\rangle\langle l|H_1|k\rangle\langle k|H_1|n\rangle}{(E_n - \varepsilon_m)(E_n - \varepsilon_l)(E_n - \varepsilon_k)} + \ldots\end{aligned}$$

Advantages and disadvantages

- The BW formulation has the advantages that the expressions given in Eqs (4) and (6) are much simpler than those produced by RS perturbation theory, and there is no need to devise a special treatment of degeneracies $\varepsilon_m = \varepsilon_n$. A disadvantage of the BW approach is that the perturbed energy appears on the righthand side of Eq. (6). This is therefore really a polynomial equation for E_n, which can be nontrivial to solve.

One has to weigh up the pros and cons of the BW and RS methods in deciding which one to use for a particular problem.

(?? maybe one day I'll understand it)

6.2.4 RS Non-Stationary Perturbation Theory

Нестационарная теория возмущений по Киселеву

Постановка задачи

При введении возмущения, зависящего от времени,

$$\hat{H} = \hat{H}_0 + \lambda V(t),$$

полагают, что в начальный момент времени t' имеем $V(t') = 0$. We are interested in determining the dynamics after the appearance of the potential.

Пусть до «включения» возмущения система находилась в одном из стационарных состояний гамильтониана $\hat{H}_0$:

$$\hat{H}_0|\mathrm{i}\rangle = E_{\mathrm{i}}^{(0)}|\mathrm{i}\rangle$$

так что $|\mathrm{i}\rangle$ - начальное (initial) состояние эволюции, которое определяет

$$|\mathrm{i}(t)\rangle_0 = U_0\left(t,t'\right)|\mathrm{i}\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_{\mathrm{i}}^{(0)}(t-t')}|\mathrm{i}\rangle,$$

где оператор эволюции для исходного гамильтониана $U_0\left(t,t'\right) = \mathrm{e}^{-\frac{1}{\hbar}\hat{H}_0(t-t')}$. При включении возмущения, зависящего от времени, оператор эволюции в общем виде принимает вид "Т-экспоненты":

$$U\left(t,t'\right) = \hat{\mathrm{T}}\exp\left\{-\frac{\mathrm{i}}{\hbar}\int\limits_{t'}^{t}\hat{H}(t)\mathrm{d}t\right\}$$

и удовлетворяет уравнению

$$i\hbar\frac{\partial U}{\partial t} = \hat{H}U,$$

И $U\left(t',t'\right) = 1$. Состояние в момент времени $t-$

$$|\mathrm{i}(t)\rangle = U\left(t,t'\right)|\mathrm{i}\rangle.$$

Представление взаимодействия

Рассмотрим эволюцию в базисе состояний "представления взаимодействия":

$$|\mathrm{i}(t)\rangle_I = U_0^{\dagger}\left(t,t'\right)|\mathrm{i}(t)\rangle \overset{\mathrm{def}}{=} U_I\left(t,t'\right)|\mathrm{i}\rangle$$

откуда

$$U\left(t,t'\right) = U_0\left(t,t'\right)U_I\left(t,t'\right).$$

Если возмущение малó, то состояние $|\mathrm{i}(t)\rangle_I$ мало отличается от начального $|\mathrm{i}\rangle$. Подставляя $U\left(t,t'\right) = U_0\left(t,t'\right)U_I\left(t,t'\right)$ в уравнение $i\hbar\frac{\partial U}{\partial t} = \hat{H}U$, находим

$$\mathrm{i}\hbar\frac{\partial U}{\partial t} = \mathrm{i}\hbar\frac{\partial U_0}{\partial t}U_I + U_0\mathrm{i}\hbar\frac{\partial U_I}{\partial t} = \hat{H}_0U_0U_I + U_0\mathrm{i}\hbar\frac{\partial U_I}{\partial t},$$

видим что вклад с $\hat{H}_0$ с обеих сторон уравнения сокращается. После умножения уравнения слева на $U_0^{\dagger}$ с учетом унитарности оператора эволюции $U_0^{\dagger}U_0 = \mathbb{1}$ получаем

$$\mathrm{i}\hbar\frac{\partial U_I}{\partial t} = \lambda V_I U_I$$

где потенциал в представлении взаимодействия

$$V_I = U_0^{\dagger}VU_0.$$

Разложение в ряд по λ решения уравнения для оператора эволюции в представлении взаимодействия

$$U_I\left(t,t'\right) = \hat{\mathrm{T}}\exp\left\{-\frac{\mathrm{i}}{\hbar}\lambda\int\limits_{t'}^{t}V_I(t)\mathrm{d}t\right\}$$

дает построение последовательных приближений по степеням константы связи $\lambda \to 0$.

Ведущее приближение

В первом порядке по λ

$$U_I(t,t') = \mathbb{1} - \frac{\mathrm{i}}{\hbar}\lambda \int\limits_{t'}^{t} V_I(t)\mathrm{d}t.$$

Пусть $|f\rangle$ - состояние из спектра исходного гамильтониана, причем $|f\rangle \neq |i\rangle$.В момент времени t эволюция этого состояния с помощью исходного оператора эволюции дает $|\mathfrak{f}(t)\rangle_0 = U_0(t,t')|\mathfrak{f}\rangle$. Значит, амплитуда вероятности найти начальное состояние в момент времени t в конечном (final) состоянии $|f(t)\rangle_0$ в ведущем порядке по константе связи равна

$$A_{\mathrm{fi}} = 0\langle \mathrm{f}(t)|\mathrm{i}(t)\rangle = \left\langle \mathrm{f}\left| U_0^{\dagger}U_0U_I \right| \mathrm{i}\right\rangle = \langle \mathrm{f}|U_I(t,t')|\,\mathrm{i}\rangle \approx -\lambda\frac{\mathrm{i}}{\hbar}\int\limits_{t'}^{t}\langle \mathrm{f}|V_I(t)|\,\mathrm{i}\rangle\,\mathrm{d}t.$$

Для матричного элемента, очевидно, имеем

$$\langle \mathrm{f}|V_I(t)|\,\mathrm{i}\rangle = \left\langle \mathrm{f}\left| U_0^{\dagger}(t,t')\,V(t)U_0(t,t')\right| \mathrm{i}\right\rangle = \langle \mathrm{f}|V(t)|\mathrm{i}\rangle \mathrm{e}^{\mathrm{i}\omega_{\mathrm{fi}}(t-t')},$$

где

$$\langle \mathrm{f}|V(t)|\mathrm{i}\rangle = V_{\mathrm{fi}}(t)$$

есть матричный элемент возмущения, и частота «перехода»

$$\omega_{\mathrm{fi}} = \frac{1}{\hbar}\left(E_{\mathrm{f}}^{(0)} - E_{\mathrm{i}}^{(0)}\right).$$

Если конечное состояние находится в дискретном спектре, то, возводя в квадрат модуль амплитуды

$$A_{\mathrm{fi}} = -\lambda\frac{\mathrm{i}}{\hbar}\int\limits_{t'}^{t} V_{\mathrm{fi}}(t)\mathrm{e}^{\mathrm{i}\omega_{\mathrm{fi}}(t-t')}\mathrm{d}t,$$

получаем вероятность перехода из начального состояния в конечное

$$W_{\mathrm{i}\to\mathrm{f}} = \frac{1}{\hbar^2}\left|\int\limits_{t'}^{t}\lambda V_{\mathrm{fi}}(t)\mathrm{e}^{\mathrm{i}\omega_{\mathrm{fi}}(t-t')}\mathrm{d}t\right|^2,$$

а в случае непрерывного спектра в конечном состоянии со спектральным параметром ν - плотность вероятности

$$\frac{\mathrm{d}W_{\mathrm{i}\to\mathrm{f}}}{\mathrm{d}\nu} = \frac{1}{\hbar^2}\left|\int\limits_{t'}^{t}\lambda V_{\mathrm{fi}}(t)\mathrm{e}^{\mathrm{i}\omega_{\mathrm{fi}}(t-t')}\mathrm{d}t\right|^2,$$

где состояния нормированы стандартным способом: $\langle\nu'|\nu\rangle = \delta(\nu'-\nu)$.

General, important questions about non-stationary RS PT

How to guess the approach to derive the non-stationary RS PT?

(??? I'll answer later)

О хронологической экспоненте

(?? где раздел, который чисто ей и посвящен??)

Введем хронологическое произведение операторов, которое часто называют также T-упорядоченным произведением операторов, или просто T-произведением. Для бозе-операторов

$$\mathrm{T}\widehat{A}(x)\widehat{B}(x') = \begin{cases} \widehat{A}(x)\widehat{B}(x') & \text{если } t > t' \\ \widehat{B}(x')\,\hat{A}(x) & \text{если } t < t' \end{cases}$$

а для ферми-операторов

$$\mathrm{T}\widehat{A}(x)\widehat{B}(x') = \begin{cases} \widehat{A}(x)\hat{B}(x') & \text{при } t > t' \\ -\widehat{B}(x')\,\widehat{A}(x) & \text{при } t < t' \end{cases}$$

(??? и почему это так???)

Relation of non-stationary PT and scattering theory

(write how exactly it is used there)

Relation of non-stationary PT and Dyson's series
(???? how they are related???)

Why does a state within a continuum have to be treated with time-dependent PT?

(???)

The point is that the state generally gets "lost" into the continuum, i.e. the true energy eigenstates have zero overlap with the original unperturbed state. For example, if we prepare an atom in an excited state but allow it to radiate into vacuum (thus introducing a continuum of states of the electromagnetic field), then no matter how we prepare the atom, the long-term probability of occupancy of the state is zero. This is true no matter how weak the perturbation is, making time-independent PT useless. (??????)

Математические указания для работы с нестационарной теорией возмущений (!?!?)

Во время использования ТВ постоянно возникают проблемы с интегралами или матрицами, так что приведем тут обзор самых основных методов по решению таких проблем.

(?? как брать эти интегралы????)

Постоянное возмущение

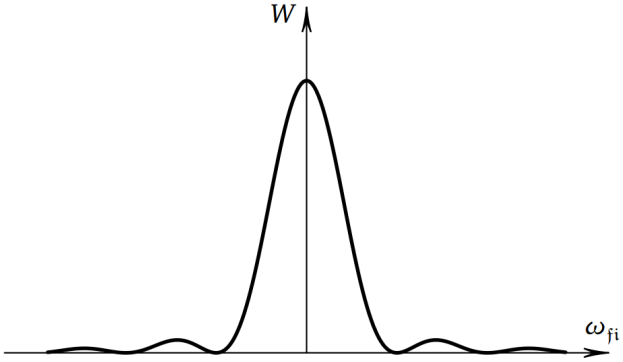
Если

$$\lambda V(t) = \bar{V}\theta(t - t'),$$

то квадрат модуля амплитуды $W_{\mathrm{i}\to\mathrm{f}} = \frac{1}{\hbar^2}\left|\int\limits_{t'}^{t} \lambda V_{\mathrm{fi}}(t)\mathrm{e}^{\mathrm{i}\omega_{\mathrm{fi}}(t-t')}\mathrm{d}t\right|^2$ равен

$$W = \left|\bar{V}_{\mathrm{fi}}\right|^2 \left(\frac{2\sin\left[\omega_{\mathrm{fi}}(t - t')/2\right]}{\hbar\omega_{\mathrm{fi}}}\right)^2,$$

характерное поведение которого на конечных временах показано на рис. 27.



Значит, постоянное возмущение с ненулевыми недиагональными матричными элементами по состояниям исходного гамильтониана за конечное время Δt приводит к переходам с частотой

$$\Delta t \cdot \omega_{\mathrm{fi}} \lesssim 1,$$

в то время как переходы с другими частотами подавлены. Если трактовать измерение спектра системы как введение малого возмущения, то, как видим, только бесконечно длительное наблюдение за стационарным состоянием позволяет избежать возбуждения других состояний, и при конечном времени измерения всегда возникает неопределенность энергии за счет переходов на другие уровни, причем имеет место соотношение неопределенности время-энергия.

При $t' \to -\infty, t \to +\infty$ возмущение действует бесконечно долго, так что амплитуда перехода

$$-\frac{\mathrm{i}}{\hbar}\bar{V}_{\mathrm{fi}} 2\pi\delta\left(\omega_{\mathrm{fi}}\right)$$

и она формально обращается в нуль при $\omega_{\mathrm{fi}} \neq 0$ на фоне вклада начального состояния, в то время как

$$2\pi\delta(\omega)\big|_{\omega\to 0} = \int\limits_{t'\to-\infty}^{t\to+\infty} \mathrm{e}^{\mathrm{i}\omega t}\,\mathrm{d}t\Bigg|_{\omega\to 0} = (t-t') \to \infty,$$

и мы получаем поправку к эволюции за счет смещения уровня

$$E_{\mathrm{i}} = E_{\mathrm{i}}^{(0)} + \bar{V}_{\mathrm{ii}},$$

так как

$$U_0\left(t,t'\right) U_I\left(t,t'\right) \mapsto \exp\left\{-\frac{\mathrm{i}}{\hbar}\left(E_{\mathrm{i}}^{(0)} + \bar{V}_{\mathrm{ii}}\right)\left(t-t'\right)\right\}.$$

При конечных временах и $\omega_{\mathrm{fi}}(t-t') \gg 1$ амплитуда перехода равна

$$A_{\mathrm{fi}} = -\frac{1}{\hbar\omega_{\mathrm{fi}}}\bar{V}_{\mathrm{fi}}\left\{1 - \mathrm{e}^{-\mathrm{i}\omega_{\mathrm{fi}}(t-t')}\right\}\mathrm{e}^{\mathrm{i}\omega_{\mathrm{fi}}(t-t')}.$$

Заметим, что в представлении взаимодействия матричные элементы операторов отличаются от матричных элементов по состояниям в представлении Гейзенберга, которое фактически используется в стационарной теории возмущений:

$$\left\langle \mathrm{f}\left|U_0^{\dagger}\left(t,t'\right)\hat{F}U_0\left(t,t'\right)\right|\mathrm{i}\right\rangle = \mathrm{e}^{\mathrm{i}\omega_{\mathrm{fi}}(t-t')}\langle \mathrm{f}|\hat{F}|\mathrm{i}\rangle,$$

что, естественно, никак не сказывается на вероятности, определяемой модулем амплитуды.

Поэтому вычисленная нами выше амплитуда может быть связана с амплитудой смешивания стационарных состояний $\tilde{A}_{\mathrm{fi}}$ согласно

$$A_{\mathrm{fi}} = \mathrm{e}^{\mathrm{i}\omega_{\mathrm{fi}}(t-t')}\tilde{A}_{\mathrm{fi}},$$

где уже

$$\tilde{A}_{\mathrm{fi}} = -\frac{1}{\hbar\omega_{\mathrm{fi}}}\bar{V}_{\mathrm{fi}}\left\{1-\mathrm{e}^{-\mathrm{i}\omega_{\mathrm{fi}}(t-t')}\right\},$$

и это-величина, которая сильно осциллирует при малом изменении интервала времени, и значит, имеет смысл взять ее среднее значение по периоду, так что экспонента «выпадает», и в среднем амплитуда не зависит от времени:

$$\bar{A}_{\mathrm{fi}} = -\frac{\bar{V}_{\mathrm{fi}}}{\hbar\omega_{\mathrm{fi}}} = \frac{\bar{V}_{\mathrm{fi}}}{E_{\mathrm{i}}^{(0)}-E_{\mathrm{f}}^{(0)}},$$

что, конечно, воспроизводит результат стационарной теории возмущений для амплитуды примеси к начальному состоянию. Поэтому критерий применимости теории возмущений в этом случае остается без изменений.

Итак, мы убедились, что подстановка постоянного возмущения согласуется с теорией возмущений в стационарном случае.

Периодическое возмущение

(?? тут же ведь и золотое правило Ферми)

Рассмотрим периодическое возмущение, равное нулю при $t = t'$,

$$\lambda V(t) = \frac{1}{\mathrm{i}}\left\{\bar{V}\mathrm{e}^{\mathrm{i}\omega(t-t')} - \bar{V}^{\dagger}\mathrm{e}^{-\mathrm{i}\omega(t-t')}\right\}, \quad \bar{V}^{\dagger} = \bar{V}, \quad V(t') = 0,$$

Амплитуда согласно общему выражению (15.40) принимает вид интерференции двух вкладов

$$A_{\mathrm{fi}} = -\mathrm{i}\left\{\frac{\bar{V}_{\mathrm{fi}}}{\hbar(\omega_{\mathrm{fi}}+\omega)}\left(1-\mathrm{e}^{\mathrm{i}(\omega_{\mathrm{fi}}+\omega)(t-t')}\right) - \frac{\bar{V}_{\mathrm{fi}}^{\dagger}}{\hbar(\omega_{\mathrm{fi}}-\omega)}\left(1-\mathrm{e}^{\mathrm{i}(\omega_{\mathrm{fi}}-\omega)(t-t')}\right)\right\},$$

формальный анализ каждого из которых вполне аналогичен рассмотрению постоянного возмущения, но физические выводы существенно отличаются.

Так, во-первых, при $|(\omega_{\mathrm{fi}} \pm \omega)(t-t')| \gg 1$ сильно осциллирующие со временем экспоненты в среднем «вымирают», и амплитуда

$$A_{\mathrm{fi}} \approx \mathrm{i}\frac{2\omega\bar{V}_{\mathrm{fi}}}{\hbar(\omega_{\mathrm{fi}}^2-\omega^2)}.$$

Она мала вдали от резонанса $\omega_{\mathrm{fi}}^2 - \omega^2 = 0$, так как $|\omega_{\mathrm{fi}}^2 - \omega^2| \sim \omega^2$ и $\left|\bar{V}_{\mathrm{fi}}\right| \ll \hbar\omega$. Во-вторых, при $\omega_{\mathrm{fi}} \pm \omega \to 0$ имеет место резонанс, который мы рассмотрим при длительном действии возмущения: $t' \to -\infty, t \to +\infty$. Тогда интегрирование в (15.40) дает

$$A_{\mathrm{fi}} = \frac{\mathrm{i}}{\hbar}\bar{V}_{\mathrm{fi}}\left\{2\pi\delta(\omega_{\mathrm{fi}}+\omega) - 2\pi\delta(\omega_{\mathrm{fi}}-\omega)\right\}.$$

Считая частоту возмущения положительной по определению, заключаем, что один из вкладов отличен от нуля, если только, когда имеет место возбуждение уровня $\omega_{\mathrm{fi}} = \omega$ - вынужденное поглощение энергии квантовой системой за счет возмущения, $E_{\mathrm{f}} = E_{\mathrm{i}} + \hbar\omega$, либо когда происходит переход с вышележащего уровня на нижележащий $\omega_{\mathrm{fi}} = -\omega$

- вынужденное излучение энергии квантовой системой, $E_\mathrm{f} = E_\mathrm{i} - \hbar\omega$. При этом мы установили, что амплитуды индуцированного поглощения и излучения по модулю равны друг другу. В случае излучения, например,

$$|A_\mathrm{fi}|^2 = \frac{1}{\hbar^2}\left|\bar{V}_\mathrm{fi}\right|^2 2\pi\delta\left(\omega_{fi}+\omega\right)2\pi\delta\left(\omega_\mathrm{fi}+\omega\right)\Big|_{\omega_\mathrm{fi}+\omega\to 0} = \frac{1}{\hbar^2}\left|\bar{V}_\mathrm{fi}\right|^2 2\pi\delta\left(\omega_\mathrm{fi}+\omega\right)\left(t-t'\right),$$

где мы опять воспользовались выражением для дельта-функции от частоты при нулевом значении аргумента через полный временной интервал действия возмущения. Поэтому имеет смысл говорить о вероятности (плотности вероятности) перехода системы за единичное время:

$$w_\mathrm{fi} = \frac{\mathrm{d}\left|A_\mathrm{fi}\right|^2}{\mathrm{d}t} = \frac{1}{\hbar}\left|\bar{V}_\mathrm{fi}\right|^2 2\pi\delta\left(E_\mathrm{f}^{(0)} - E_\mathrm{i}^{(0)} + \hbar\omega\right),$$

причем мы внесли $\hbar$ под знак дельта-функции. Если конечное состояние находится в непрерывном спектре со спектральным параметром $\nu = \nu\left(E_f^{(0)}\right)$, то получаем «золотое правило Ферми» для дифференциальной вероятности перехода за единичное время:

$$\mathrm{d}w_\mathrm{fi} = \frac{1}{\hbar}\left|\bar{V}_\mathrm{fi}\right|^2 2\pi\delta\left(E_\mathrm{f}^{(0)} - E_\mathrm{i}^{(0)} + \hbar\omega\right)\mathrm{d}\nu\left(E_\mathrm{f}^{(0)}\right)$$

где $\mathrm{d}\nu\left(E_\mathrm{f}^{(0)}\right)$ - дифференциальная плотность состояний с заданной энергией конечного состояния.

Подчеркнем, что согласно формулам (15.49), (15.50) бесконечно длительное воздействие периодического возмущения приводит к точному закону сохранения энергии для уровней исходной системы в смысле квантового характера поглощения и излучения энергии.

Периодическое возмущение: Details and related concepts

Золотое правило Ферми: More discussion

$$dw_\mathrm{fi} = \frac{1}{\hbar}\left|\bar{V}_\mathrm{f}\right|^2 2\pi\delta\left(E_\mathrm{f}^{(0)} - E_\mathrm{i}^{(0)} + \hbar\omega\right)d\nu\left(E_\mathrm{f}^{(0)}\right)$$

(just tell again and more, what is the sense and how to work with it, because it is an important rule)

Золотое правило ферми at the second order

(?????. нужно будет - освоюсь с этим)

О ширине распада (???)

(?? зачем оно тут написано вообще??)

Если вычислить интегральную вероятность перехода из одного состояния в другое за единицу времени $w_{fi} = \int \mathrm{d}w_\mathrm{fi}$, то можно ввести величину τ с размерностью времени $w_\mathrm{fi} = \frac{1}{\tau}$.

Тогда, если рассмотреть распад в ансамбле из N идентичных квантовых систем в момент времени t, то за время $\mathrm{d}t$ вероятность распада

$$-\frac{\mathrm{d}N(t)}{N(t)} = \frac{\mathrm{d}t}{\tau},$$

что легко интегрируется, и

$$N(t) = N_0 \mathrm{e}^{-\frac{1}{\tau}}.$$

Согласно этому уравнению τ называют временем жизни системы, если имеет место индуцированное излучение и распад, или временем возбуждения, если происходит не распад, а вынужденное поглощение (в этом случае число систем в ансамбле с исходным состоянием также экспоненциально убывает). При этом совершенно ясно, что по прошествии времени τ вероятность индуцированного излучения или поглощения становится близка к единице. Поэтому логично считать критерием применимости теории возмущений для периодического возмущения не малость вероятности перехода за время наблюдения, а несколько иной показатель. Именно, единственным условием, которое должно с необходимостью выполняться в ходе вывода выражения для вероятности перехода в единицу времени, будет достаточная длительность воздействия возмущения, много большая, чем период колебаний возмущения. Этого всегда можно достичь, если только время жизни уровня много больше периода колебаний возмущения:

$$\tau \gg \frac{1}{\omega}$$

Поскольку в резонансе частота колебаний связана с разностью энергий уровней соотношением $\hbar\omega = |\hbar\omega_{\mathrm{fi}}| = \left|E_{\mathrm{f}}^{(0)} - E_{\mathrm{i}}^{(0)}\right| = \Delta E$, условие применимости расчета вероятности перехода за счет периодического возмущения (15.54) можно представить в виде

$$\Gamma \ll \Delta E,$$

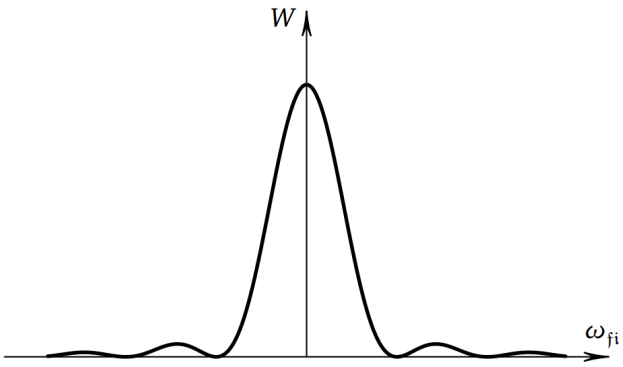
где

$$\Gamma = \frac{\hbar}{\tau}$$

называют шириной перехода.

В задаче с постоянным возмущением мы видели, что дельта-функция, отвечающая закону сохранения энергии, возникает в пределе бесконечно длительного воздействия возмущения. В случае же конечного времени воздействия имеется конечная ширина распределения по энергии, которая связана с временем воздействия соотношением неопределенности время-энергия.

Этот вывод, очевидно, остается справедлив и для периодического возмущения: просто центр распределения на рис. 27 смещается с нуля к величине $\Delta E/\hbar$.



Поскольку характерное время перехода равно τ, соответствующая неопределенность в значении энергии перехода есть $\hbar/\tau = \Gamma$. Поэтому, например, ширина перехода определяет в процессе вынужденного излучения точность определения энергии распадающегося уровня, т. е. ширину уровня.

Другое условие применимости теории возмущений - сходимость ряда по константе связи λ. Степень сходимости можно установить, только вычислив следующую по λ поправку к ширине перехода $\Gamma^{(2)}$ и убедившись, что $\Gamma^{(2)} \ll \Gamma$.

Мгновенное включение возмущения

(??? here, there is a very special theory, and I'll think more about it later again)

При рассмотрении постоянного возмущения мы полагали, что в момент включения возмущения от нулевого значения до $\bar{V}$ состояние системы точно совпадало с одним из квантовых уровней невозмущенной, исходной системы с гамильтонианом $\hat{H}_0$. Однако это предположение нуждается в более детальном исследовании, так как необходимо установить точность такого приближения, учитывая фактическую конечность интервала времени изменения потенциала, и обсудить возможную связь с соотношением неопределенности время-энергия.

Для простоты обозначений будем считать, что в начальный момент времени $t' = 0$ возмущение быстро возрастает от нуля до величины $\bar{V}$ за малое время δt:

$$\lambda V(t) = \bar{V}(s), \quad t = \delta t \cdot s, s \in [0, 1].$$

Гамильтониан как функция параметра s равен

$$\hat{H}(s) = \hat{H}_0 + \bar{V}(s).$$

Оператор эволюции в первом приближении по малому $\delta t-$

$$U(\delta t) = \mathbb{1} - \frac{\mathrm{i}}{\hbar} \int\limits_0^1 \hat{H}(s)\delta t \, \mathrm{d}s = \mathbb{1} - \frac{\mathrm{i}}{\hbar}\delta t \bar{H},$$

где мы ввели «среднее значение» гамильтониана

$$\bar{H} = \int\limits_0^1 \hat{H}(s)\mathrm{d}s.$$

Теперь сразу видно, что

$$\lim_{\delta t \to 0} U(\delta t) = \mathbb{1},$$

т. е. при мгновенном изменении потенциала начальное состояние действительно не изменяется.

Вычислим вероятность найти систему в момент времени δt в состоянии, отличном от начального:

$$w = \sum_{\mathbf{f} \neq \mathrm{i}} |\langle \mathbf{f}|U(\delta t)|\mathrm{i}\rangle|^2 = \sum_{\mathbf{f} \neq \mathrm{i}} \left\langle \mathrm{i} \left| U^\dagger(\delta t) \right| \mathbf{f} \right\rangle \langle \mathbf{f}|U(\delta t)|\mathrm{i}\rangle.$$

(???? tell better, why do we use exactly this approach???)

В силу полноты базиса

$$\sum_{\mathrm{f} \neq \mathrm{i}} |\mathrm{f}\rangle\langle \mathrm{f}| = \mathbb{1} - |\mathrm{i}\rangle \left\langle \mathrm{i} \right| = \bar{P}_\mathrm{i}, \quad \bar{P}_\mathrm{i} \left| \mathrm{i} \right\rangle = 0, \quad \langle \mathrm{i}|\bar{P}_\mathrm{i} = 0, \quad \bar{P}_\mathrm{i}^2 = \bar{P}_\mathrm{i}, \quad \bar{P}_\mathrm{i}^\dagger = \bar{P}_\mathrm{i},$$

здесь $\bar{P}_\mathrm{i}$ это проектор на пространство, ортогональное исходному состоянию $|\mathrm{i}\rangle$, так что

$$w = \left\langle \mathrm{i} \left| U^\dagger(\delta t) \bar{P}_\mathrm{i} U(\delta t) \right| \mathrm{i} \right\rangle.$$

В ведущем приближении использование ортогональности дает

$$\langle \mathrm{i}|U^\dagger(\delta t)\bar{P}_\mathrm{i} = \frac{\mathrm{i}}{\hbar}\delta t \left\langle \mathrm{i}\right|\bar{H}\bar{P}_\mathrm{i}, \quad \bar{P}_\mathrm{i}U(\delta t)\left|\,\mathrm{i}\right\rangle = -\frac{\mathrm{i}}{\hbar}\delta t\bar{P}_\mathrm{i}\bar{H}|\mathrm{i}\rangle,$$

и значит,

$$w = \frac{1}{\hbar^2}(\delta t)^2 \left\langle \mathrm{i}\right|\bar{H}\bar{P}_\mathrm{i}\bar{H}\left|\,\mathrm{i}\right\rangle = \frac{1}{\hbar^2}(\delta t)^2 \left\{\langle \mathrm{i}|\bar{H}\bar{H}|\mathrm{i}\rangle - \langle \mathrm{i}|\bar{H}|\mathrm{i}\rangle^2\right\}.$$

Но выражение в фигурных скобках есть не что иное, как квадрат флуктуации $\delta\bar{H}$ среднего значения гамильтониана,

$$w = \frac{1}{\hbar^2}(\delta t \cdot \delta\bar{H})^2,$$

поэтому вероятность возбуждения состояний, отличных от начального, пренебрежимо мала, $w \ll 1$, если

$$\delta t \cdot \delta\bar{H} \ll \hbar$$

Ясно, что флуктуация среднего значения гамильтониана $\delta\vec{H} \sim \delta E$ определяется величиной малого возмущения $\delta E \sim V$.

Мгновенное включение возмущения: Related concepts

Relation to time-energy uncertainty

(????????????? is it related or not???)

Согласно соотношению неопределенности время-энергия при флуктуации энергии на величину δE состояние, а значит, его волновая функция существенно, т. е. физически значимо, изменится за время

$$\Delta t \geqslant \frac{\hbar}{\delta E}$$

Таким образом, включение возмущения можно считать мгновенным, если состояние не успевает измениться за время δt,

$$\delta t \ll \Delta t \sim \frac{\hbar}{\delta\bar{H}},$$

т. е. интервал времени для инициации возмущения много меньше характерного времени изменения волновой функции за счет изменения энергии.

О нестационарной теории возмущений в вырожденном случае (???)

(вопрос, что делать в этом случае? пока не знаю, потом подумаю.)

Typical illustrative examples of non-stationary PT

О возбуждении осциллятора

Если действует на осциллятор $F\hat{x}e^{-t^2/\tau^2}$, то

$$V_{nm}(t) = -Fe^{-t^2/\tau^2}\langle n|\hat{x}|m\rangle = -\frac{Fe^{-t^2/\tau^2}}{\sqrt{2m\omega}} \cdot \begin{cases} \sqrt{n}, & m = n-1 \\ \sqrt{n+1}, & m = n+1 \end{cases}$$

А формула второго порядка для перехода в состояния, невозможные по первому

$$\partial_t\psi_2^{(2)}(t) = -i\int\limits_{-\infty}^{t} d\tau_1 V_{21}^{(I)}(\tau_1)\,\psi_1^{(1)}(\tau_1) = (-i)^2\int\limits_{-\infty}^{t} d\tau_1 V_{21}^{(I)}(\tau_1)\int\limits_{-\infty}^{\tau_1} d\tau_2 V_{10}^{(I)}(\tau_2)$$

(вроде этого достаточно для задачи, потом проверю, пока не понял теорию возмущений еще)

6.2.5 Perturbation Theory in QFT: Overview

Perturbation theory is so popular and so very powerful, because it is applied in QFT. It is a topic for a whole section, but here we will discuss just main ideas and applications.

(???I'll write it here after I write it in the note of QFT)

6.3 Perturbation theory: Well-known Special Cases and Features

6.3.1 Perturbation Theory in the Continuous Spectrum

Рассмотрим задачу рассеяния в случае, когда к рассеивающему потенциалу добавляется малый возмущающий потенциал. Найдем изменение амплитуды рассеяния по теории возмущений.

Scattering on a finite nuclei

В качестве примера изучим рассеяние заряженных частиц на атомных ядрах и вычислим добавку к амплитуде кулоновского рассеяния из-за конечности ядра.

Пусть гамильтониан системы равен

$$H = H_0 + H',$$

где H' - малая добавка, причем известно решенне задачи с гамильтонианом H_0:

$$H_0\varphi_p = E_p\varphi_p.$$

Граничные условия, налагаемые на φ_p в случае задачи рассеяния (непрерывный спектр), могут быть двух типов:

$$\varphi_p^{\pm} \longrightarrow e^{ipr} + \frac{f_{\pm}}{r}e^{\pm ipr}.$$

Из них физический смысл имеют лишь функции φ_p^+, соответствующее расходящейся сферической волне, однако для вспомогательных целей бывают удобны и Φ_p. Каждая из систем функций φ_p^+ или φ_p^- является полной ортогональной системой, т. е.

$$\int \varphi_p^{+*}\varphi_{p'}^{+}dr = \int \varphi_p^{-*}\varphi_{p'}dr = (2\pi)^3\delta\left(p - p'\right)$$

Требуется найти решение уравнения Шредингера

$$H\Psi_p = E_p\Psi_p,$$

или

$$\left(H_0 - E_p\right)\Psi_p = -H'\Psi_p.$$

Решение уравнения (2.1) будем искать в виде суммы решения невозмущенной задачи $(H_0 - E_p)\Psi_p = 0$, т. е. φ_p^+, и добавки, которую удобно разложить по собственным функциям φ_p^- невозмущенной задачи, т. е.

$$\Psi_p = \varphi_p^+ + \int \frac{dp'}{(2\pi)^3}C_{pp'}\varphi_{p'}$$

(можно было бы сделать разложение и по φ_p^+, но мы увидим далее, что разложение по функциям φ_p^- удобнее).

Для того чтобы описывать рассеяние, Ψ_p должна удовлетворять граничному условию

$$\Psi_p \underset{r\to\infty}{} e^{ipr} + \frac{f}{r} e^{ipr}.$$

Функция φ_p^+ удовлетворяет этому условиют

$$\varphi_p^+ \underset{r\to\infty}{\longrightarrow} e^{ipr} + \frac{f_0}{r} e^{ipr}$$

(f_0 - амплитуда рассеяния невозмущенной задачи). Поэтому должно быть

$$\int \frac{dp'}{(2\pi)^3} C_{pp'} \varphi_{p'} \underset{r\to\infty}{\longrightarrow} \frac{f_1}{r} e^{ipr}.$$

Определим $C_{pp'}$. Умножим (2.1) слева на $\varphi_{p'}^{-*}$. Учитывая $I_0 \varphi_{p'} = E_{p'} \varphi_{p'}^-$и интегрируя по T, получаем

$$(E_{p'} - E_p) \int \varphi_{p'}^{-*} \Psi_p dr = -\int \varphi_{p'}^{-*} H' \Psi_p dr$$

или, сокращенно,

$$(E_{p'} - E_p) (\varphi_{p'} (\Psi_p) = - (\varphi_{p'} |H'| \Psi_p)$$

При $|\boldsymbol{p}| \neq |\boldsymbol{p}'|$ согласно (2.2) получаем

$$\left(\varphi_{p'}^- | \Psi_p\right) = \left(\varphi_{p'}^- | \varphi_p^+\right) + \int \frac{dp''}{(2\pi)^3} C_{pp''} \left(\varphi_{p'}^- | \varphi_{p''}^-\right) = \int \frac{dp''}{(2\pi)^3} C_{pp''} \delta\left(p' - p''\right) (2\pi)^3 = C_{pp'}$$

Здесь использовано то, что при $|p| \neq |p'|$ функции $\varphi_{p'}$ и φ_p^+ортогональны. Из (2.4) находим:

$$C_{pp'} = \frac{(\varphi_{\bar{p}'} |H'| \Psi_p)}{E_p - E_{p'}}.$$

Следовательно,

$$\Psi_p = \varphi_p^+ + \int \frac{dp'}{(2\pi)^3} \frac{\left(\varphi_{p'}^- |H'| \Psi_p\right)}{E_p - E_{p'}} \varphi_{p'}^-$$

Интегральное уравнение (2.5) эквивалентно дифференциальному уравнению (2.1). Запись уравнения для Ψ_p в интегральной форме имеет то преимущество, что в этой форме удобно получать последовательные приближения. Именно:

$$\begin{aligned}
\Psi_p^{(0)} &= \varphi_p^+, \\
\Psi_p^{(1)} &= \int \frac{dp'}{(2\pi)^3} \frac{\left(\varphi_{p'} |H'| \varphi_p^+\right)}{E_p - E_{p'}} \varphi_{p'}^- \\
\Psi_p^{(2)} &= \int \frac{dp'}{(2\pi)^3} \frac{\left(\varphi_{p'} |H'| \Psi_p^{(1)}\right)}{E_p - E_{p'}} \varphi_{p'}^-
\end{aligned}$$

и т. д.

Подынтегральное выражение (2.5) [или (2.6)] имеет особую точку при $|\boldsymbol{p}| = |p'|$. Мы увидим, что способ обхода особой точки определяет асимптотический вид Ψ_p, т. е. ставит граничные условия. Мы покажем, что именно указанный на рис. 17 способ обхода (а не обход сверху и не интеграл в смысле главного значения) дает граничные условия (2.3).

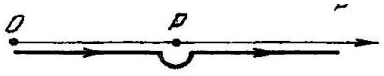


Рис. 17.

Перейдем к вычислению интеграла в выражении (2.6) для $\Psi_{p'}$ ири $r \longrightarrow \infty$. Функция $\varphi^-_{p'}$при $r \to \infty$ имеет вид

$$\varphi_{\overrightarrow{p}} \overrightarrow{r \to \infty} e^{ip'rx} + \frac{f_i^-}{r} e^{-ip'r},$$

где

$$x = \cos \angle (p'r)\,.$$

Первое слагаемое этого выражения приводит к интегралу в (2.6) вида

$$\int\limits_{-1}^{1} F(x) e^{tp'rx} dx.$$

Интегрируя по частям, имеем

$$\int\limits_{-1}^{1} F(x) e^{ip'rx} dx = \frac{1}{ip'r} e^{ip'rx} F(x)\Big|_{-1}^{1} - \frac{1}{ip'r} \int\limits_{-1}^{1} e^{ip'rx} \frac{dF}{dx} dx \underset{r\to\infty}{\approx} \frac{F(1)e^{ip'r} - F(-1)e^{-ip'r}}{ip'r}.$$

Гокажем, что часть этого выражения, содержащая $e^{-ip'r}$, исчезает в пределе $r \longrightarrow \infty$ при интегрировании по dp'. Нужно оценить интеграл

$$\frac{1}{r} \int\limits_{\Omega} \frac{dp'}{E_p - E_{p'}} e^{-ip'r} \Phi\,(p')\,.$$

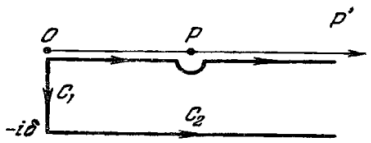


Рис. 18.

Контур интегрирования изображен на рис. 17. Заменим контур интегрирования на $C_1 + C_2$ (рис. 18), взяв δ достаточно малым, чтобы между старым и новым контуром не было особых точек. Тогда величина интеграла (2.7) не изменится. $= e^{-i\xi r} \cdot e^{-\hat{\partial} r}$ иле по $C_2 p' = \xi - i\delta, \quad \delta > 0$, поэтому $e^{-ip'r} =$ (2.7), и, следовательно, при $r \longrightarrow \infty$ весь интеграл по C_2 экспоненциально мал. На участке $C_1 p' = -it$, и получается интеграл

$$\frac{1}{r} \int\limits_{0}^{\delta} \frac{e^{-rt}}{E_p - E_{it}} (\mathrm{D}(t) dt.$$

При $r \longrightarrow \infty$ интервал для t, существенный в подынтегральном выражении (2.8), порядка $[0, 1/r]$, следовательно, E_{it} мало в этом интервале, $E_{it} \ll E_p$. Поэтому интеграл (2.8) порядка $\frac{1}{r} \int\limits_0^\delta e^{-rt} dt \sim \frac{1}{r^2}$, т. е. мал степенным образом.

По тем же соображениям мала степенным образом и часть интеграла в (2.6), содержащая слагаемое $\frac{f_i^-}{r} e^{-ip'\tau}$ асимптотического выражения для $\varphi_{p'}$. В этом и состоит преимущество базисных функций φ_p^- по сравнению с φ_p^+.

Следовательно, в (2.6) остается лишь интеграл с $e^{ip'r}$. Для его вычисления выбираем контур, изображенный на рис. 19.

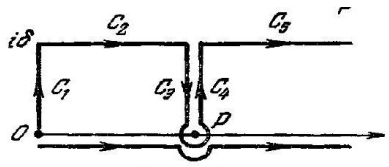


Рис. 19.

Как и для интеграла с $e^{-ip'r}$, в этом случае интеграл по C_2+C_5 будет экспоненциально мал, а по C_1 - мал степенным образом. Интегралы по C_3 и C_4 взаимно уничтожатся. Следовательно, весь интеграл сводится к вычету в точке $p'=p$:

$$\Psi_p = \varphi_p^+ + 2\pi i \frac{2\pi p'^2}{(2\pi)^3} \cdot \frac{\left(\varphi_{p'}!H'|\varphi_p^+\right)}{dE_p/dp} \frac{e^{ip'r}}{ip'r},$$

где $p' = p\frac{r}{r}$. Окончательно:

$$\Psi_p = \varphi_p^+ - \frac{p}{2\pi v}\left(\varphi_{p'}\left|H'\right|\varphi_p^+\right)\Big|_{p'=p\frac{r}{r}} \cdot \frac{e^{ipr}}{r}.$$

Итак, Ψ_p имеет нужную асимптотику:

$$\Psi_p = e^{ipr} + \frac{(f_0+f_1)}{r} e^{ipr},$$

причем

$$f_1 = -\frac{p}{2\pi v}\left(\varphi_{p'}^-\left|H'\right|\varphi_p^+\right)\Big|_{p'=p\frac{r}{r}}$$

Для нерелятивистских частиц можно заменить $p/v = m$.

В случае свободного движения φ_p^+и $\varphi_{\bar{p}}^-$- плоские волны, $f_0 = 0$, и мы получаем амплитуду рассеяния в так называсмом борновском приближении:

$$f_1 = -\frac{p}{2\pi v}\int HI'(r')\, e^{iqr'}dr',$$

где

$$q = p - p\frac{r}{r}$$

передаваемый импульс при рассеянии: $|q| = 2p\sin\frac{\theta}{2}$, а θ - угол рассеяния.

критерий применимости теории возмущений в непрерывном спектре

Найдем критерий применимости теории возмущений в непрерывном спектре. Принцип отыскания критерия любого приближенного расчета состоит в том, что приближенно вычисленная физическая величина должна быть велика по сравнению с поправко к ней от следующего порядка приближения.

В рассматриваемом случае дополнительная амплитуда рассеяния равна

$$-\frac{m}{2\pi}\int \varphi_{p'} H' \Psi_p dr'$$

В первом порядке теории возмуценин $\Psi_p = \varphi_p^+$и

$$f_1 = -\frac{m}{2\pi}\int \varphi_{p'} H' \varphi_p^+ dr'$$

Во втором порядке теории возмущений

$$f_2 = -\frac{m}{2\pi}\int \varphi_p \overline{p'} H' \Psi_p^{(1)} dr' \sim m\int \varphi_{p'} H' \frac{f_1}{r'} e^{ipr'} dr'$$

Условие $f_2/f_1 \ll 1$ служит критерием применимости решения в рассматриваемой задаче.

Iусть a - порядок величины области пространства, в которой возмущаюшее поле $H'(r)$ заметно отлично от нуля. Рассмотрим сначала случай $pa \leqslant 1$. Тогда функции $\varphi_p^{\pm}(a)$ по порядку величины равны единице. Следовательно, амплитуда f_1 порядка $H'(a)a^3$ и слабо зависит от угла рассеяния. Поэтому $f_2/f_1 \sim H' f_1 a^2/f_1 \sim H' a^2$ и критерий теории возмущений имеет вид

$$H' a^2 \ll 1$$

Рассмотрим теперь случай $pa \geqslant 1$. Более подробно этот случай исследован в 3.1. Рассеяние в этом предельном случае больших энергий резко анизотропно и направлено вперед. Действительно, в выражении (2.9) величина

$$\varphi_{p'}^{*}\varphi_p^{+} \sim e^{iqr} \sim e^{ipa\sin\frac{\theta}{2}}$$

сильно осциллирует при $pa \gg 1$ для всех углов рассеяния θ, кроме $\theta \leqslant 1/pa \ll 1$. Для углов рассеяния $\theta \leqslant 1/pa$ величина $\varphi_{p'}^{-*}(a)\varphi_p^{+}(a)$ по порядку величины равна 1 и амплитуда рассеяния имеет оценку

$$f_1(\theta) \underset{\theta\leq 1/pa}{\sim} H'(a)a^3$$

Для углов $\theta \gg 1/pa$ амплигуда $f_1(\theta)$ сущиествнно уменьиается нз-3а осцилляцни волновых функций $\varphi_p^{\pm}$.

6.3.2 Scattering of Charged Particles on Nuclei

Рассеяние заряженных частиц на атомном ядре

В качестве примера рассмотрим рассеяние заряженных частиц (электронов или μ имезонов) на атомном ядре. Будем считать, что заряд ядра равномерно распределен по его объему. Тогда потенциальная энергия частицы:

$$V = \begin{cases} -\frac{Z}{R}\left(\frac{3}{2} - \frac{1}{2}\frac{r^2}{R^2}\right), & 0 < r < R \\ -\frac{Z}{r} & , \quad r > R. \end{cases}$$

Здесь Z - заряд ядра, R - радиус ядра. Следовательно,возмущение имеет вид

$$H' = \begin{cases} -\frac{Z}{R}\left(\frac{3}{2} - \frac{1}{2}\frac{r^2}{R^2}\right) + \frac{Z}{r}, & 0 < r < R \\ 0 & r > R. \end{cases}$$

Согласно (2.9) дополнительная амплитуда рассеяния равнз

$$f_1 = -\frac{1}{2\pi}\int \varphi_{p'}^{-*} H' \varphi_p^{+} dr \approx -\frac{1}{2\pi}\varphi_{p^*}{}^{*}(0)\varphi_p^{+}(0)\int H' dr$$

Действительно, H' изменяется на расстоянии порядка R, а φ_p - на расстоянии порядка $1/p$. Для не слишком больших скоростей элегтронов $pR \ll 1$ (в атомных единицах $R \leq 10^{-4}$). Гоэтому в зыражении для f_1 функции $\varphi_{p'}^{-}$и φ_p^{+} можно выносить из-под знака интеграла в точке $r = 0$.

Вычисление дает

$$\int H' dr = \frac{2\pi Z R^2}{5}.$$

Следовательно,

$$f_1 = -\frac{ZR^2}{5}\varphi_p^{-*}(0)\varphi_p^{+}(0).$$

Кулоновские нерелятивистские волновые функции $\varphi_p^{\pm}(0)$ равны:
для поля отталкивания:

$$\varphi_p^{\pm}(0) = \frac{1}{\sqrt{(2\pi)^3}} e^{-\pi/2p}\Gamma\left(1 \pm \frac{i}{p}\right),$$

для поля притяжения

$$\varphi_p^{\pm}(0) = \frac{1}{\sqrt{(2\pi)^3}} \epsilon^{\pi/2p}\Gamma\left(1 \mp \frac{i}{p}\right),$$

где $\Gamma\left(1 \pm \frac{i}{p}\right)$ - гамма-функция. Окончательно получаем:

$$f_1 = -\frac{1}{80\pi^3}\frac{ZR^2}{a_0} e^{\pm 2\pi/p}\Gamma^2\left(1 \pm \frac{i}{p}\right),$$

где знак минус относится к потенциалу отталкивания, а плюс - к потенциалу притяжения; a_0-боровский радиус.

Дифференциальное сечение рассеяния $d\sigma/d\Omega$ равно

$$d\sigma/d\Omega = |f_0 + f_1|^2,$$

где f_0 - амплитуда кулоновского рассеяния. Поскольку f_1 не зависит от угла рассеяния, а f_0 убывает с увеличением угла рассеяния, то учет конечности ядра существен при больших углах рассеяния.

Критерий применимости теории возмущений в этом случае ($pR \ll 1$)-это $H'R^2 \ll 1$ или $2R^2 \ll 1$; он выполняется для всех реальных ядер.

Мы не интересовались рассеянием налетающей частицы на атомных электронах. Амплитуды такого рассеяния можно вычислить, зная атомный форм-фактор. При не слишком малых углах рассеяния влиянием атомных электронов можно пренебречь.

6.3.3 Perturbation of Boundary Conditions and Levels of a Deformed Nucleus

Теория

В этом разделе рассматривается случай, когда возмущение наложено на граничные условия. Преобразованне координат позволяет привести граничные условия к невозмущенному виду. Однако оно изменяет выражение для гамильтониана системы. Это изменение гамильтониана и есть возмущающий потенциал, влияние которого можно рассмотреть с помощью обычной теории возмущений. Теория поясняется на примере расчета одночастичных энергетических уровней деформированного ядра.

Пусть нам известно решение стационарной (или нестационарноӈ) задачи с гамильтонианом $H(x)$ и граничным условием на некоторой поверхности S_0:

$$\alpha\Psi + \beta\Psi'|_{S_0} = 0.$$

Требуется найти решение задачи с тем же гамильтонианом $H(x)$, но с граничным условием

$$\alpha\Psi + \beta\Psi'|_S = 0,$$

причем поверхность S близка к S_0 (эта близость и есть малый параметр в задаче). Для рсшсния задачи следует найти такое преобразование координат $x_i = f_i\left(x'_j\right)$, что $S(x) = S_0\left(x'\right)$, Т. е. в новых переменных уравнение поверхности ирежнее. Иными словами, если уравнение поверхности S_0 есть $\Phi_0\left(x_j\right) = 0$, а $S - \Phi\left(x_j\right) = 0$, то должно быть

$$\Phi\left(f_i\left(x'_j\right)\right) = \Phi_0\left(x'_j\right).$$

Гамильтониан $H\left(x_i\right) = H\left(f_i\left(x'_j\right)\right)$ в новых переменных изменяется. Мы можем запииать его в виде

$$H\left(x'_j\right) + H'\left(x'_i\right),$$

где $H'\left(x'_j\right) = H\left(f_i\left(x'_j\right)\right) - H\left(x'_j\right)$ и есть возмунение. Далее применгма уже обытная тсорня возмущений.

Энергетические уровни деформированного ядра

Пусть известны стационарные уровни энергии в сферическом ящике, а нужно найти их в эллипсоидальном ящике (стенки считаем бесконечно высокими). Уравнение поверхности S_0 имеет вид

$$\Phi_0\left(x_j\right) = 0: \quad \sum_{i=1}^{3} x_i^2 - R^2 = 0,$$

а уравнение поверхности S есть

$$\Phi\left(x_j\right) = 0: \quad \sum_{j=1}^{3} \frac{x_j^2}{a_j^2} - 1 = 0.$$

Введем новые переменные:

$$x_j = \frac{a_j x'_i}{R}.$$

Тогда $\Phi\left(f_i\left(x'_j\right)\right) = \Phi_0\left(x'_j\right)$. При этом изменяется оператор кинетической энергии частицы:

$$T\left(x_i\right) = -\frac{1}{2M}\sum_{i=1}^{3}\frac{\partial^2}{\partial x_i^2} = -\frac{R^2}{2M}\sum_{i=1}^{3}\frac{1}{a_i^2}\frac{\partial^2}{\partial x_i'^2}.$$

Следовательно, возмущение имеет вид

$$H'\left(x'_i\right) = -\frac{1}{2M}\sum_{i=1}^{3}\left(\frac{a^2}{R^2} - 1\right)\frac{\partial^2}{\partial x_i'^2}.$$

Оно малб, если все a_i близки к R.

Рассмотрим эллипсопда.тьную деформацию ядра, считая эллипсоид двухосным (с полуосями a и b). Параметром деформации называется величина

$$\beta = 2\frac{a-b}{a+b}.$$

Считаем, что объем ядра не меняется при его деформации, т. е. $ab^2 = R^3$. Если написать $a = R(1+\delta), b = R\,(1-\delta_1)$, где $\delta, \delta_1 \ll 1$, то в первом приближении из $ab^2 = R^3$ получим $\delta - 2\delta_1 = 0$, т. е.

$$\beta = 2\frac{R\,(1+2\delta_1) - R\,(1-\delta_1)}{2R} \approx 3\delta_1,$$

или

$$a \approx R\left(1 + \frac{2}{3}\beta\right)$$
$$b \approx R\left(1 - \frac{1}{3}\beta\right)$$

Тогда возмущение H' принимает следующий вид:

$$H' = -\frac{1}{2M}\left\{\left[\frac{R^2}{R^2\left(1+\frac{2}{3}\beta\right)^2} - 1\right]\frac{\partial^2}{\partial z^2} + \left[-\frac{R^2}{R^2\left(1-\frac{1}{3}\beta\right)^2} - 1\right]\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\right\} \approx$$
$$\approx -\frac{\beta}{3M}\left(\Delta - 3\frac{\partial^2}{\partial z^2}\right).$$

Пусть ε^0_{nlj} - энергия частиц без учета деформации ядер (от магнитного квантового числа она не зависит в силу сферической симметрии поля). С учетом деформации в первом порядке теории возмущений получаем

$$\varepsilon_{nljm} = \varepsilon^0_{nlj} + \left(\varphi^{(0)}_{nljm}\,|H'|\,\varphi^{(0)}_{nljm}\right).$$

В результате расıета находим

$$\varepsilon_{nljm} = \varepsilon^0_{nlj}\left[1 + \beta\left(\frac{m^2}{j(j+1)} - \frac{1}{3}\right)\right].$$

Зависимость ε_{nljm} от β схсматически изображенана рис. 20.

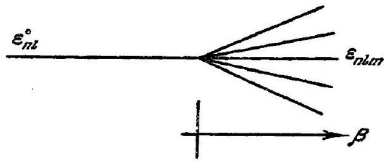


Рис. 20.

Заметим, что $\frac{1}{2j+1}\sum_{nijm} = \varepsilon^0_{nlj}$, т. е. центр тяжести мультиплета не смещается при деформации ядра.

3 ад ач а. Вычислить ε_{nln} В квазиклассицеском приближении.

6.3.4 Sudden Perturbations and Ionization in Decay and Nuclear Impact

Теория

В рассматриваемых до сих пор примерах малым пара. метром задачи было относительное изменение гамильтониана системы. Изучим случай, когда малым параметром является время действия возмущения, но само возмущение не мало.

Ионизация при β-распаде-один из примеров такого возмущения. В этом случае скорость β-распадного электрона много больше скоростей атомных электронов. Поэтому изменение заряда ядра-внезапное событие для них. Другой пример-ионизация при ударе быстрой частицы о ядро. В этом случае внезапным событием для атомных электронов служит отдача ядра.

Рассмотрим систему, волновая функция которой подчиняется уравнению Шредингера $i\frac{\partial\Psi}{\partial t} = H\Psi$ с гамильтонианом

$$H = \begin{cases} H_1(r), & t < 0, \\ H_2(r), & t > \tau. \end{cases}$$

Предположим, что гамильтониан системы сильно изменяется за короткое время τ. Введем полную систему функциія гамильтониана H_2:

$$H_2\varphi_n^{(2)} = \varepsilon_n^{(2)}\varphi_n^{(2)}$$

и разложим реиение задачи Ψ по функіиям $\Phi_n^{(2)}$:

$$\Psi(t) = \sum_n a_n(t)\varphi_n^{(2)}e^{-i\varepsilon_n^{(2)}t}$$

Запишем гамильтониан H в виде $H = H_2 + (H - H_2) = H_2 + V$. Тогда

$$i\frac{\partial\Psi}{\partial t} = i\sum_n \varphi_n^{(2)}e^{-i\varepsilon_n^{(2)}t}\left(\frac{da_n}{dt} - i\varepsilon_n^{(2)}a_n\right)$$
$$H\Psi = \sum_n a_n(t)e^{-i\varepsilon_n^{(2)}t}\left(\varepsilon_n^{(2)}\varphi_n^{(2)} + V\varphi_n^{(2)}\right)$$

откуда

$$i\frac{da_n}{dt} = \sum_m V_{nm}e^{-i\left[\varepsilon_m^{(2)} - \varepsilon_n^{(2)}\right]t}a_m(t).$$

Этот результат мог быть получен и без вычислений. Если временно обозначить $b_n(t) = a_n(t)e^{-i\varepsilon_n^{(2)}t}$, то фактически разложение $\Psi(t) = \sum\limits_n b_n(t)\varphi_n^{(2)}$ означает переход от координатного к энергетическому представлению гамильтониана H_2. Уравнение Шредингера в новом представлении имеет такой вид:

$$i\frac{\partial b_n}{\partial t} = \sum_m \left[\varepsilon_n^{(2)}\delta_{nm} + V_{nm}\right]b_m$$

откуда сразу же получаем уравнение (2.11).

Интегрируя полученное уравнение, имеем

$$a_n(t) - a_n(0) = -i\sum_m \int_0^t V_{nm}a_m(t)e^{-i\left[\varepsilon_m^{(2)} - \varepsilon_n^{(2)}\right]t}$$

Матричный элемент V_{nm} обращается в нуль при $t \gg \tau$. Предположим, что $\left(\varepsilon_n^{(2)} - \varepsilon_m^{(2)}\right)\tau \ll 1$. Тогда экспонента под интегралом приближенно равна единице. Следовательно, для того чтобы пользоваться последовательными приближениями, должно выполняться условие $V\tau \ll 1$ (возмущение не является малым, но оно действует короткое время).

В нулевом приближении из (2.12) имеем $a_n^{(0)}(t) = a_n(0)$. Заменяя в правой части уравнения (2.12) в первом приближении $a_m(t)$ на $a_m(0)$, получим

$$a_n^{(1)}(t) = -i\sum_m \int_0^t \left(\varphi_n^{(2)}|V|\varphi_m^{(2)}\right) a_m(0)dt$$

Так как

$$\sum_m a_m(0)\varphi_m^{(2)} = \Psi(0),$$

то в первом приближении находим

$$a_n^{(1)}(t) = -i\int_0^t \left(\varphi_n^{(2)}|V|\Psi(0)\right) dt.$$

Предположим, что начальное состояние $\Psi(0)$ было одной из собственных функций H_1, т. е.

$$\Psi(0) = \varphi_{n_0}^{(1)} = \sum a_n(0)\varphi_n^{(2)}.$$

Следовательно, $a_n(0) = \left(\varphi_{n_0}^{(1)}|\varphi_n^{(2)}\right)$. Итак, в нулевом приближении вероятность перехода в состояние $\varphi_n^{(2)}$ есть

$$W_{nn_0} = \left|\left(\varphi_{n_0}^{(1)}|\varphi_n^{(2)}\right)\right|^2.$$

В пространстве векторов $\Psi(t)$ с базисом φ_n внезапное возмущение соответствует сильному изменению базиса: $\varphi_n^{(1)} \longrightarrow \varphi_n^{(2)}$, при малом изменении волновой функции: $\Psi(t) \approx \Psi(0)$.

Ионизация атомов при β-распаде

Расчет ионизации атома при β-распаде сильно упрощается, если использовать тот факт, что скорость β-распадного электрона много больше скоростей атомных электронов. Покажем, что ионизация вызывается изменением заряда ядра, а непосредственным взаимодействием атомного и β-распадного электронов можно пренебречь.

Сначала оценим вероятность электронного перехода, вызываемого непосредственным взаимодействием. Согласно теории возмущений она равна

$$W = \frac{1}{\hbar}\left|\int_0^\infty V_{nn_0}e^{i\omega_{nn_0}t}dt\right|^2.$$

Здесь V_{nn_0} - матричный элемент энергии взаимодействия, а ω_{nn_0} - частота перехода.

Оценим это выражение. Величина ω_{nn_0} имеет порядок атомных частот. Время пролета β-распадного электрона τ много меньше атомных периодов, т. е. $\omega_{nn_0}\tau \ll 1$. Поэтому в (2.14) можно заменить $e^{i\omega_{nn_0}t} \longrightarrow 1$. Взаимодействие $V\beta$-электрона атомным электроном

имеет порядок величины e^2/a, где a - величина порядка атомных размеров. Так как при β-распаде электрон вылетает из атома со скоростью порядка скорости света c, то время вылета $\tau \sim a/c$. Следовательно, вероятность W имеет оценку:

$$W \sim \frac{1}{\hbar^2} V^2 \tau^2 \sim \frac{1}{\hbar^2} \left(\frac{e^2}{a} \frac{a}{c} \right)^2 \sim \left(\frac{e^2}{\hbar c} \right)^2 \ll 1.$$

Вычислим теперь вероятность ионизации вследствие изменения заряда ядра. Как мы только что видели, волновая функция атомных электронов мало меняется за время вылета β-распадного электрона. Поэтому вероятность ионизации электрона, находившегося в состоянии Ψ_0^Z в поле ядра с зарядом Z, согласно (2.13) равна

$$W_{0,E} = \left| \left(\Psi_0^Z | \Psi_E^{Z+1} \right) \right|^2.$$

Здесь Ψ_E^{Z+1} - волновая функция вылетевшего электрона с энергией $E > 0$ в поле ядра с зарядом $Z + 1$. Полная вероятность ионизации из-за изменения заряда ядра равна

$$W_0 = \int_0^\infty W_{0,E} dE.$$

Оценим (2.16). Для этого разложим функцию $f(Z_1, Z_2) = \left(\Psi_0^{Z_1} | \Psi_E^{Z_2} \right)$ в ряд по разности $Z_1 - Z_a$:

$$f(Z_1, Z_2) \approx \left(\Psi_0^{Z_1} | \Psi_E^{Z_1} \right) + (Z_1 - Z_2) \left. \frac{\partial f}{\partial Z_1} \right|_{z_1 = z_2} = (Z_1 - Z_2) \left. \frac{\partial f}{\partial Z_1} \right|_{Z_1 = z_2}.$$

Производная $\left. \frac{\partial f}{\partial Z_1} \right|_{Z_1 = Z_2} = \left(\Psi_E^{Z_1} | \frac{\partial \Psi_0^{Z_1}}{\partial Z_1} \right) \sim \frac{1}{Z_1}$. Следовательно, $\left(\Psi_0^{Z_1} | \Psi_E^{Z_2} \right) \sim \frac{Z_1 - Z_2}{Z_1} = \frac{1}{Z_1}$, т.е.

$$W_0 \sim \frac{1}{Z^2}.$$

Итак, относительное влияние непосредственного взаимодействия имеет порядок величины

$$\left(\frac{Ze^2}{\hbar c} \right)^2 = \left(\frac{Z}{137} \right)^2 \ll 1.$$

Оно выполняется для всех ядер, кроме самых тяжелых.

Из (2.14) можно сделать заключение о правилах отбора для рассматриваемого процесса. В случае ионизации внутренних оболочек самосогласованное поле, в котором движется электрон, можно считать сферически симметричным, следовательно, $\Psi = R_{nl}(r) Y_{lm}(\theta, \varphi)$. Подставляя это Ψ в (2.14), получим правила отбора:

$$l_1 = l_2, \quad m_1 = m_2.$$

Для наружных оболочек эффективный заряд Z, действующий на атомные электроны, порядка 1. Следовательно, согласно (2.17) и вероятность ионизации $W_k \sim 1$. Это подтверждается экспериментами по накоплению положительных ионов при $\beta\pm$-распаде, Вероятность ионизации можно вычислить до конца для K - и L-оболочек. В этих случаях существенна область вболизи ядра, где функции Ψ_0^Z и Ψ_E^{Z+1} можно считать водородоподобными (пользование водородоподобными функциями вносит погрешность порядка $1/Z$).

Вероятность ионизации быстро убывает, когда энергия вылетающего электрона становится много больше потенциала ионизации. Действительно, в этом случае функция

Ψ_E^{Z+1} много раз осциллирует на атомных размерах ининтеграл (2.15) мал. Таким образом, вылетающие электроны имеют энергию между нулем и величиной порядка потенциала ионизации.

Получим вероятность ионизации для K-электрона, когда энергия вылетающего атомного электрона много больше потенциала ионизации. Радиальная волновая функция R_E^{Z+1} при больших энергиях должна совпадать с радиальной функцией свободной частицы:

$$R_E^{Z+1} \sim \frac{1}{r}\sqrt{\frac{\overline{2}}{\pi k}}\sin kr.$$

$E \to \infty$

Здесь $k = \sqrt{2E}$. Функция R_E нормирована на интервал энергий

$$\int\limits_0^\infty R_E R_E \cdot r^2 dr = \delta\left(E - E'\right).$$

Следовательно,

$$W_{1E} = \left|\int\limits_0^\infty R_1^Z R_E^{Z+1} r^2 dr\right|^2_{E\to\infty} \approx \frac{2}{\pi k}\left|\int\limits_0^\infty R_1^Z \sin krr dr\right|^2$$

Для K-электрона $R_1^Z = 2Z^{3/2}e^{-Zr}$. Следовательно, нужно вычислить интеграл $I = \int\limits_0^\infty re^{-Zr}\sin krdr\mathrm{np}k \longrightarrow \infty$. Интегрируя его по частям, получаем $I \approx 2Z/k^3$ (интеграл вычпслялся в 1.1, стр. 19, и на стр. 53).

Итак, при $E \geqslant Z^2$ вероятность ионизации K-электрона приближенно равна:

$$W_{1E} \approx \frac{8Z^3}{\pi k}\left(\frac{2Z}{k^3}\right)^2 = \frac{32}{\pi}\frac{Z^5}{k^7} \text{ или } \underset{E\to\infty}{W_{1E}} \approx \frac{2\sqrt{2}}{\pi}\frac{Z^5}{E^{7/2}}.$$

Ионизация атомов при ядерных реакциях

При ядерных столкновениях с большой передачей энергии должна пронсходить ионизация атомов отдачи. Если скорость, приобретенная ядром, невелика, то ядро успевает увлечь электроны, и ионизация происходит только в наружных, слабо связанных оболочках. Наоборот, при больших скоростях ядро вылетает из оболочки, не увлекая ее за собой.

Вычислим вероятность ионизации при ударе нейтрона о ядро. Времь! соударения нейтрона с ядром $\tau \sim R/v_\mathrm{f}$, где R - радиус ядра, $v_\mathrm{н}$ - скорость нейтрона. Это время много меньше электронных периодов τ. ГПоэтому за время столкновения электронная волновая функция практически не меняется.

Если обозначить через v_s скорость, приобретенную ядром, то смещение l ядра за время соударения имеет порядок величины $l \sim v_\mathrm{g}\tau \sim \frac{v_\mathrm{G}}{v}R \sim \frac{M_\mathrm{H}}{M_\mathrm{g}}R < R$, т. е. l много меньше размеров электронной оболочки. Следовательно, ядро практически не смещается за время удара.

Перейдем к системе координат, в которой ядро после соударения покоится. Тогда волновая функция начального состояния преобразуется в выражеиие

$$\Psi_0 \longrightarrow e^{iv_0\Sigma r_i}\Psi_0\left(r_1, r_2, \ldots\right),$$

где ϑ - скорость отдачи ядра. Это выражение проще всего получить, разлагая Ψ_0-функцию по плоским волнам и сдвигая каждый из импульсов этих волн на величинну

σ. Пусть $\Psi_1(\boldsymbol{r}_1, \tau_2, \ldots)$ обозначает конечное состояние атома. Вероятность возбуждения согласно (2.13) равна

$$W = \left|\left(\Psi_1 \left| e^{iv_1 \Sigma r_i} \right| \Psi_0\right)\right|^2.$$

Критерий применимости этой формулы: $\tau \ll \tau$. Его можно записать также в виде $\frac{R}{v} \ll \frac{a}{v_э}$ или $v \gg \frac{R}{a} v_э$, где a - величина порядка размеров изучаемой оболочки.

Из выражения (2.18) можно гоолучит формулу для вероятности перехода одного фиксированного электрона. Так как взанмодействне между электронами мало по сравнению с полем ядра при $Z \gg 1$, то

$$W = W_1 W_2,$$

где W_1 - вероятность перехода рассматрнваемого электрона, а W_2 - вероятность возбуждения всех остальных электронов.

Суммируя по всем конечным состояниям, получим $\sum\limits_1 W_1 = 1, \sum\limits_2 W_2 = 1$. Следовательно, вероятность перехода рассматриваемого электрона из состояния ψ_0 в состояние ψ_n ра ВНа

$$W = W_1 \sum_2 W_2 = 1 \int \psi_n e^{i\psi_1 r} \psi_0 dr \Bigg|^2$$

Если скорость ядра много меньшге скорости электрона но $\boldsymbol{v} \gg v_a \frac{R}{a}\big)$, то экспоненту в (2.19) можно разложить в ряд. Нулевой член разложения исчезает из-за ортогональности функций Ψ_0 и Ψ_n. Пусть скорость v_{nuc} направлена по оси $\boldsymbol{z}$. Тогда

$$W = v_a^2 \left|(\Psi_n|z|\Psi_0)\right|^2.$$

Наоборот, если $v_a \geqslant v_3$, то экспонента $e^{iv\Sigma r_i}$ в (2.18) [или (2.19)] быстро осциллирует. Следовательно, вероятность перехода W не мала, только если $\Psi_1 \sim e^{-iw\Sigma r_i}$, т. е., когда электроны в новой системе движутся со скоростью - $\boldsymbol{r}_я$ В лабораторной системе координат это соответствует тому, что электронная оболочка не увлекается ядром при ударе.

Если скорость ядра $\boldsymbol{v}$ больше скорости внешних электронов, но меньше скорости внутренних электронов, т. е. $1 < v_я < Z$, то внутренние оболочки атома увлекаются ядром, а наружные - нет. Заряд получающегося иона равен по порядку величины числу электронов на наружных оболочках.

Такне соображения позволяют оценить заряд осколков при делении. Заряд определяется как чнсло электронов со скоростями, менышими чем скорость осколка (см. стр. 85).

Для атома водорода и для внутренних оболочек другнх атомов вычисления можно довести до конца. Вероятность ионизации и возбуждения для этих случаев приводится в задачах.

Оценим полную вероятность возбуждения и ионизации W при $v \ll 1$.Π_3(2.20) находим

$$W = C_1 v_{r_3}^2$$

где C_1 - число порядка единицы. Из решения задачи 6 следует, что вероятность атому водорода остаться в основном соттоянии равна

$$W_{00} = \frac{1}{\left(1 + \frac{1}{4} v_9^2\right)^4}.$$

Отсюда находим, что для атома водорода $C_1 = 1$.

Передача энергии при вылете кванта из ядра молекулы (эффект Мёссбауэра)

Предположим, что квант с энергией $\hbar\omega$ вылетает из ядра, входящего в молекулу. Если ω мало, то молекула получает слабый толчок и воспринимает отдачу как единое целое. Если $\hbar\omega$ велико, то ядро вылетает из молекулы происходит возбуждение системы (те же соображения применимы и к металлам: при малом ω отдачу воспринимает вся кристаллическая решетка).

Оценим время вылета τ кванта из ядра; τ - это время пролета пакета радиуса $\lambda = c/\omega$ через область ядра, т. е. $\tau \sim \lambda/c = 1/\omega$. Эта оценка неверна при $\lambda < R$, где R - радиус ядра, т. е. при $\omega > c/R \sim 137 \cdot 10^4 .27$ зв ~ 0 Мэв.

Время τ ничтожно по сравнению с временами, характеризующими колебания и вращения молекулы. Следовательно, Ψ-функция молекулы не успевает измениться за время вылета кванта. Задача напоминает задачу об ионизации при ядерных реакциях. Волновая функция молекулы в начальный момент после испускания кванта имеет вид

$$\Psi' = \Psi\left(r_1, r_2, ...\right) e^{iMvr_1},$$

где v - скорость отдачи, r_1 - радиус-вектор ядра, из которого вылетел квант, M - масса атома. Функция Ψ описывает основное состояние молекулы. Вероятность того, что молекула останется невозбужденного, равна

$$W_0 = \left|\left(\Psi_0 \left| e^{iMvr_1} \right| \Psi_0\right)\right|^2.$$

Если $Mvr_1 \ll 1$, то $W_0 \sim 1$, т. е. отдача воспринимается всей молекулой, возбуждения нет. Оценим частоту γ-квана ω, начиная с которой возбуждаются колебательные степени свободы молекулы. Как мы увидияi, амплитуда колебаний чмеет порядок величины $1/\sqrt[4]{M}$. Поэтому в (2.21)$r_1 \sim 1/\sqrt[4]{M}$. Следовательно, для того чтобы колебания не возбуждались, должно быть $Mv\frac{1}{\sqrt[4]{M}} \ll 1$. Так как импульс ядра $p_{\text{и}} = Mv$ равен импульсу кванта $\hbar\omega/c$, это условие означает, что $\hbar\omega/c \ll \sqrt[4]{M}$, чли $\omega \ll 137\sqrt[4]{M}$ (в атомных единицах ; в эв:

$$\omega \ll 137\sqrt[4]{100 \cdot 1840} \cdot 27 \ \ni \approx \sim 70\kappa \ni \ э$$

(здесь взято ядро с $A \sim 100$).

Критерий применимостя (2.21):

$$\hbar\omega \gg \hbar\omega_{\text{кол}} \ \sim 1/\sqrt{M} \sim \frac{27}{\sqrt{100 \cdot 1840}} \sim 0,06 \geqslant 6,$$

где $\omega_{\text{кол}}$ - колебательная частота молекулы.

Оненим теперь частоту кванта, начиная с которой возбуждаются вращательные стенени свободы молекулы. Для элого рассмотрим плоский ротатор. Его волновая функция $\psi_m = e^{im+\varphi}$, Вероятность перехода из состояния ψ_0 В состояние ψ_m согласно (2.21) равна

$$w_{m0} = \left|\int \Psi_m e^{iMvr} \psi_0 dr\right|^2 \sim \left|\int_0^{2\pi} e^{im\hbar\varphi + iMva\cos\varphi} d\varphi\right|^2$$

где a - величина порядка размеров молекулы.

Следовательно, для того цтобы вращательнье уровни не возбуждались, необходимо, чтобы момент колнчества движения $\sim$ M?a, сообиценный молекуле квантом, был много меньше момента количества двнжения ротатора m$\hbar$. В эпом случае из (2.22) находим $w_{m0} \ll_{m\neq 0} 1$. Для наинизшего возбуiкдения ($m = 1$) получасм

$$Mva \leqslant h \quad \text{или} \quad \frac{h\omega}{c} a \leqslant h,$$

откуда $h\omega \ll c = 137 \cdot 27$ эв ~ 4 кэв.

6.3.5 Collisions in Perturbation Theory: Typical Examples

(?? maybe I'll move later it to the section on atomic physics, but currently I am fine that it is here)

MK-ch2.3.1

Убедиться в том, что отдача ядра не существенна для ионизации атома при β-распаде.

MK-ch2.3.2

Вычислить вероятность возбуждения K-электрона при β-распаде в состояние дискретного спектра с главным квантовым числом n и вероятность того, что электрон останется в s-состоянии ($Z \gg 1$).

О т в г.

$$W_{1n}^{n\neq 1} = 2^6 \frac{(n-1)^{2n-4}}{(n+1)^{2n+4}} n^5 \frac{1}{Z^2}, \quad W_{11} = 1 - \frac{3}{4}\frac{1}{Z^2}.$$

MK-ch2.3.3

Используя метод Томаса - Ферми, оценить заряд осколков при делении ядра, считая его равным числу электронов со скоростью, меньшей скорости осколков.

О т в е Т.

$$Z_{\text{оск}} \sim 8.$$

MK-ch2.3.4

Найти вероятность перехода K-электрона при β-распаде в состояние непрерывного спектра с энергией E и полную вероятность ионизации ($Z \gg 1$).

О т в е г.

$$W_{1E} = 2^7 \frac{e^{-\frac{4Z}{k} \operatorname{arctg} \frac{k}{Z}}}{\left(1 + \frac{k^2}{Z^2}\right)^4 \left(1 - e^{-\frac{2\pi Z}{k}}\right)} \frac{1}{Z^2}, \quad W_1 = \frac{0,32}{Z^2}.$$

MK-ch2.3.5

Оценить ионизацию атома из-за магнитного взаимодействия налетающего нейтрона с электроном.

Or в е г.

$$\frac{W_{\text{MarH}}}{W} \leqslant \left|\frac{V_{\text{MarH}}\tau}{v_{\text{H}}}\right|^2 \sim \left|\frac{\mu_{\text{H}} u_3}{a^3}\frac{R}{v_{\text{H}}^2}\right|^2 \ll \left|\frac{1}{M_{\text{H}}c^2}\frac{1}{R}\right|^2 \sim 10^{-7}.$$

MK-ch2.3.6

Определить вероятность того, что при ударе нейтрона о ядро атома водорода электрон останется в основном состоянии.

О т в Т

$$W_{11} = \frac{1}{\left(1 + \frac{1}{4}v_\Omega^2\right)^4}.$$

MK-ch2.3.7

Вычислить вероятность ионизации атома водорода при столкновении его с нейтроном.

О т в r.

$$W_{0k}dk = 2^8 \frac{v_g^2\left(v_g^2 + \frac{1}{3}k^2 + \frac{1}{3}\right)e^{-\frac{2}{k}\operatorname{arctg}\frac{2k}{v_g^2-k^2+1}}}{\left[(v_s+k)^2+1\right]\left[(v_n-k)^2+1\right]\left[1-e^{-2\pi/k}\right]}kdk.$$

MK-ch2.3.8

Вычислить полную вероятность ионизации атома водорода при столкновении его с нейтроном, когда скорость ядра много меньше скорости электрона.

Or B e T.

$$W_1 = 0,28v_s^2$$

6.3.6 Perturbation Theory in the Case of Close Levels

Теория

(??? отсюда пока ничего не усвоил, но вроде как тут все просто)

Рассмотрим систему с двумя близкими уровнями, на которую наложено возмущение (случай большего числа близких уровней внесет лищь алгебраические усложнения). Пусть возмущение достаточно мало́, так что можно пренебречь примесью состояний с далекими энергиями, между тем как состояния с близкими энергиями смешиваются сильно.

Решение уравнения Шредингера

$$(H_0 + H')\,\Psi == E\Psi,$$

где H' - возмущение, следует искать в виде суперпозиции состояний, соответствующих близким уровням:

$$\Psi = C_1\Psi_1 + C_2\Psi_2,$$

причем функции $\Psi_{1,2}$ удовлетворяют невозмущенному уравнению

$$H_0\Psi_{1,2} = \varepsilon_{1,2}\Psi_{1,2.}$$

Коэффициенты C_1, C_2 в (2.72) имеют одинаковый порядок величины.

Найдем энергетические уровни возмущенной системы. Для этого запишем уравнение Шредингера в представлении C_1, C_2 :

$$\left.\begin{aligned}(E-\varepsilon_1)\,C_1 &= H'_{11}C_1 + H'_{12}C_2,\\ (E-\varepsilon_2)\,C_2 &= H'_{21}C_1 + H'_{22}C_2.\end{aligned}\right\}$$

Коэффициенты C_1, C_2 отличны от нуля, если детерминант системы (2.73) равен нулю, т. е.

$$\begin{vmatrix} E-\varepsilon_1-H'_{11} & -H'_{12} \\ -H'_{21} & E-\varepsilon_2-H'_{22} \end{vmatrix} = 0.$$

Из (2.74) получаем

$$(E-\varepsilon_1-H'_{11})(E-\varepsilon_2-H'_{22}) - |H'_{12}|^2 = 0,$$

откуда

$$E = \frac{\varepsilon_1+\varepsilon_2+H'_{11}+H'_{22}}{2} \pm \sqrt{\frac{(\varepsilon_1+\varepsilon_2+H'_{11}+H'_{22})^2}{4} - (\varepsilon_1+H'_{11})(\varepsilon_2+H'_{22}) + |H'_{12}|^2}.$$

Обозначая $\varepsilon_1 + H'_{11} = \tilde{\varepsilon}_1, \varepsilon_2 + H'_{22} = \tilde{\varepsilon}_2$, окончательно находим

$$E = \frac{\tilde{\varepsilon}_1+\tilde{\varepsilon}_2}{2} \pm \frac{1}{2}\sqrt{(\tilde{\varepsilon}_1-\tilde{\varepsilon}_2)^2 + 4|H'_{12}|^2}.$$

В случае применимости обычной теории возмущений: $|H'_{12}| \ll |\varepsilon_1 - \varepsilon_2|$, из (2.75) получаем

$$E \approx \frac{1}{2}\left\{\tilde{\varepsilon}_1+\tilde{\varepsilon}_2 \pm \left[(\tilde{\varepsilon}_1-\tilde{\varepsilon}_2) + \frac{2|H'_{12}|^2}{\tilde{\varepsilon}_1-\tilde{\varepsilon}_2}\right]\right\},$$

или

$$E^{(1)} \approx \varepsilon_1 + H'_{11} + \frac{|H'_{12}|^2}{\varepsilon_1-\varepsilon_2},$$
$$E^{(2)} \approx \varepsilon_2 + H'_{22} - \frac{|H'_{12}|^2}{\varepsilon_1-\varepsilon_2},$$

что и следовало ожидать. При $H' \longrightarrow 0$ величина $E^{(1)} \to \varepsilon_1$, а $E^{(2)} \to \varepsilon_2$. Наоборот, в случае $\varepsilon_1 = \varepsilon_2 = \varepsilon$ из (2.75) имеем

$$E = \varepsilon + \frac{H'_{11}+H'_{22}}{2} \pm |H'_{12}|.$$

Заметим, что если для какоголибо возмущения, зависящего от - ξ параметра, $H'_{12} \neq 0$, то уровни $E^{(1)}$ $E^{(2)}$, как функции параметра хи не пересекаются, так как в (2.75) $\sqrt{(\tilde{\varepsilon}_1-\tilde{\varepsilon}_2)^2 + 4|H_{12}|^2} > 0$. Уровни энергии при этом имеют вид, изображенный на рис. 22.

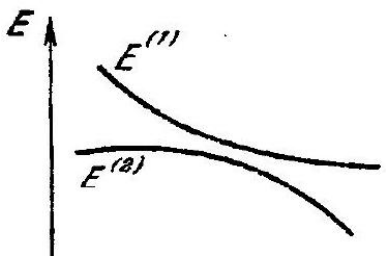


Рис. 22.
(????? подумаю про это больше, пока не очень понял)

Частица в периодическом потенциале

Рассмотрим, как изменяется движение свободной частицы при наложении периодического возмущения

$$V = V_0 \left(e^{ikx} + e^{-ikx}\right).$$

Волновая функция невозмущенной задачи имеет вид $\Psi_p = e^{ipx}$. Среднее значение V по любому невозмущенному состоянию равно нулю, а отличны от нуля лишь матричные элементы $V_{p,p-k} = V_{p,p+k} = V_0$ (длину ямы считаем равной 1). В обычной теории возмущений сдвиг энергетических уровней равен

$$E_p = \varepsilon_p + \frac{V_0^2}{\varepsilon_p - \varepsilon_{p-k}} + \frac{V_0^2}{\varepsilon_p - \varepsilon_{p+k}},$$

где $\varepsilon_p = p^2/2M$. Однако это выражение применимо лишь в случае $V_0 \ll |\varepsilon_p - \varepsilon_{p-k}|$, т. е. когда p не близко $\kappa \pm k/2$. (!?!?!??! поч?? переучу!)

Если $p \to k/2$, то состояния Ψ_p и Ψ_{p-k} имеют близкие энергии, и волновую функцию частицы нужно искать в виде

$$\Psi = C_1\Psi_p + C_2\Psi_{p-k}$$

(при $p \to -k/2 \quad \Psi = C_1\Psi_\mu + C_2\Psi_{p+k}$). Из
(2.75) для собственных значений энергии получаем выражение:

$$E_p = \frac{\varepsilon_p + \varepsilon_{p-k}}{2} \neq \sqrt{\frac{\left(\varepsilon_p - \varepsilon_{p-k}\right)^2}{4} + V_0^2}$$

Выбор знака в (2.77) определяется тем условием, чтобы при $|\varepsilon_p - \varepsilon_{p-k}| \gg V_0$ энергия E_p стремилась к ε_p. Так как при $p < k/2$ величина $\sqrt{\left(\varepsilon_p - \varepsilon_{p-k}\right)^2} = |\varepsilon_p - \varepsilon_{p-k}| = \varepsilon_{p-k} - \varepsilon_p$, а при $p > k/2\sqrt{\left(\varepsilon_p - \varepsilon_{p-k}\right)^2} = \varepsilon_p - \varepsilon_{p-k}$, то для $p < k/2$ в (2.77) нужно взять один знак корня, а при $p > k/2$ - другой.

Для E_p получается разрывная кривая, изображенная на рис. 23.

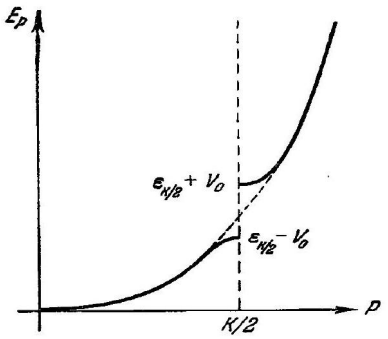


Рис. 23.

При этом величина разрыва равна $E_{k/2+0} - E_{k/2-0} = 2V_0$.

Таким образом, при наложении периодического потенциала в спектре свободных частиц появляется щель (!!!! укажу это в 1 части!!!), Отсюда понятно возникновение запрещенных зон в металлах для электронов (правда, там нужно рассматривать трехмерный случай).

Кз (2.77) следует, что $\left.\frac{dE}{dp}\right|_{p=k/2} = 0$, т. е. групповая скорость тастицы на краю зоны ($p = k/2$) равна нулю. Это соответствует тому, что на краю зонь волновая функция частицы есть стоячая, а не бегущая волна.

Штарк-эффект в случае близких уровней

Рассмотрим систему с двумя близкими уровнями, на которую наложено однородное электрическое поле $V(x) =$. Определим, как изменяется энергия системы в этом поле. Среднее значение V по любому состоянию с определенной четностью равно нулю (дипольный момент $d_x = \int \Psi^*_\lambda(r) x \Psi_\lambda(r) dr$ при замене переменной интегрирования $r \to -r$ переходит в $-d_x$, т. е. $d_x = 0$). Для энергетических уровней системы в поле $E_{1,2}$ получаем:

$$E_{1,2} = \frac{\varepsilon_1 + \varepsilon_2}{2} \pm \sqrt{\frac{(\varepsilon_1 - \varepsilon_2)^2}{4} + |V_{12}|^2}.$$

Рассмотрим, например, состояния $2s_{1/2}$ и $2p_{1/2}$ атома водорода. Они обладают одинаковой энергией (если не учитывать лэмбовского смещения). Расщепление такого дублетного уровня при наложении электрического поля линейно по полю и равно $E_2 - E_1 = 2\,|V_{12}|$.

Вычислим V_{12}. Для состояния $2s_{1/2}$ волновая функция равна $R_{20}(r)\frac{1}{\sqrt{4\pi}}$, а для состояния $2p_{1/2}$ равна $R_{21}\sqrt{\frac{3}{4\pi}}\cos\theta$. $R_{nl}(r)$ - радиальные кулоновские функции. Следовательно, $V_{12} = -\delta\,(R_{20}|r|R_{21})\,\frac{\sqrt{3}}{4\pi}\int \cos^2\theta d\Omega = -\frac{\delta}{\sqrt{3}}\,(R_{20}|r|R_{21})$.

Матричные элементы динольного момента для кулоновских радиальных функций табулированы. В частности, $(R_{20}|r|R_{21}) = 3\sqrt{3}$. Следовательно, $|V_{12}| = 30°$.

Итак, расщепление дублета $2s_{1/2}, 2p_{1/2}$ в слабом электрическом поле в атомных единицах равно 6&.

Заметим, что уровень $2p_{s/2}$ имеет ту же четность, "ito и $2p_{1/2}$. Поэтому $\int \Psi_{2p_{3/2}} x \Psi_{2p_{1/2}} dr = 0$. Следовательно, эти уровни в нашем линейном по полю приближении не расщепляются. Для их расщепления нужно рассматривать суперпозицию трех состояний $-2s_{1/2}, 2p_{1/2}, 2p_{z/2}$.

Для всех других атомов, кроме атома водорода, расщепление термов квадратично по полю: $E = E_0 + \frac{1}{2}\ \propto^2$. Действительно, уровни сложных атомов не вырождены относительно орбитального квантового числа l, т. е. нет состояний с близкими энергиями, которые перемешивались бы в слабом электрическом поле.

Изменение времени жизни состояния $2s_{1/2}$ атома водорода во внешнем электридеском поле

B атоме водорода состояние $2s_{1/2}$ имеет большое время жизни. Действительно, переход $2s_{1_{12}} \to 1s_{1/2}$ может происходить лишь с испусканием двух γ-квантов. Время жизни состояния $2s_{1/2}$ по отношению к этому переходу порядка 1/7 сек. Кроме того, возможен еще дипольный переход $2s_{1/2} \to 2p_{1/2}$ (энергии обоих состояний различаются из-за лэмбовского сменения). Оценим вероятность этого перехода.

В (1.4) мы нашли, что вероятность дипольного перехода w $\sim \omega^3/c^3$, где ω-частота перехода. Разность энергий $\omega = E_{2s_{1/2}} - E_{2p_{1/2}}$ имеет порядок $1/c^3$ (см. стр. 63). Следовательно, w $\sim 1/c^{12}$. В атомных единицах $c \approx 137$, следовательно, $\nsim 10^{-24}$, т. е. время жизни состояния $2s_{1/2}$ по отношению к переходу $2s_{1/2} \to 2p_{1/2}$ порядка $10^{24}\tau$, где $\tau_{\text{ат}}$ - атомное время $\sim 10^{-16}$ сек. Utак, рассматриваемое время $\sim 10^8$ сек. Мы видим, что переход $2s_{1/2} \to 1s_{1/2}$ все же веронтнее, чем переход $2s_{1/2} \to 2p_{1/2}$.

При наложении вненнего поля состояние атома будет суперпозицией состояний $2s_{1/2}$ и $2p_{1/2}$. Но как только атом перейдет в состояние $2p_1/2$ он моментально (за время $\tau \sim 10^{-9}$ сек) совершит дипольный переход: $2p_{1/2} \to 1s_{1/2}$. Мы видим, что время жизни состояния 25%/2 резко изменяется при наложении электрического поля. Итак, будем считать $\Psi =$

$C_1 e^{-i\varepsilon_1 t}\psi_1 + C_2 e^{-i\varepsilon_2 t}\psi_2$, где индекс 1 соответствует состоянию $2s_{1/2}$, а индекс $2-2p_{1/2}$. Для величин C_1, C_2 имеем уравнения

$$i\dot{C}_1 = V_{12}C_2 \exp\left[i\left(\varepsilon_1 - \varepsilon_2\right)t\right]$$
$$i\dot{C}_2 = -i\frac{1}{\tau}C_2 + V_{21}C_1 \exp\left[-i\left(\varepsilon_1 - \varepsilon_2\right)t\right]$$

Здесь $V = -6x$. Матричные элементы $V_{11} = V_{22} = 0$. Затухания состояния $2s_{1/2}$ со временем $\sim 1/7$ сек не учитываем. Даже в отсутствие внешнего поля C_2 не является постоянной: $C_2^{(0)} \sim \exp(-t/\tau)$ из-за взаимодействия с полем излучения. Здесь т имеет порядок времени жизни дипольного состояния ($\tau \sim 10^{-9}$ сек). $C_1^{(0)}$ считаем постоянной, поскольку время затухания состояния $2s_{1/2}$ очень велико. Обозначим $C \equiv C_2 \exp\left(i\varepsilon_{12}t\right)$, где $\varepsilon_{12} \equiv \varepsilon_1 - \varepsilon_2$ - лэмбовское сменение. Тогда из (2.79) имеем:

$$i\dot{C}_1 = V_{12}C, \quad i\dot{C} = V_{21}C_1 - \left(\varepsilon_{12} + i/\tau\right)C.$$

Исключая C_1, получтем $\ddot{C} + \left(-i\varepsilon_{12} + \frac{1}{\tau}\right)\dot{C} + \left|V_{12}^2\right|^2 = 0$. Ищем решение уравнения в виде $C = Ae^{i\omega t}$. Тогда получаем

$$\omega^2 - \omega\left(\frac{i}{\tau} + \varepsilon_{12}\right) - \left|V_{12}\right|^2 = 0,$$

что дает два комплексных корня для ω, причем $\varepsilon_{12} \sim 1/\tau$. В начальный момент времени $C_1(t=0) = 1, C(t=0) = 0$. Начальное условие для C будет выполнено, если искать C в виде $C = a\left[\exp\left(i\omega^{(1)}t\right) - \exp\left(i\omega^{(2)}t\right)\right]$. Из (2.80) находим

$$C_1 = \frac{i\dot{C} + \left(\varepsilon_{12} + i/\tau\right)C}{V_{21}} = \frac{a}{V_{21}}\left\{\left(\frac{i}{\tau} + \varepsilon_{12} - \omega^{(1)}\right)\exp\left(i\omega^{(1)}t\right) + \left(\frac{i}{\tau} - \varepsilon_{12} + \omega^{(2)}\right)\exp\left(i\omega^{(2)}t\right)\right\}.$$

Величина a определяется из условия $C_1(t=0) = 1$:

$$a = V_{21}\left(\frac{2i}{\tau} + \omega^{(2)} - \omega^{(1)}\right)^{-1}.$$

Из уравнения (2.81.) найдем частоты $\omega^{(1)}, \omega^{(2)}$;

$$\omega = \frac{1}{2}\left(\varepsilon_{12} + \frac{i}{\tau}\right) \pm \sqrt{\frac{1}{4}\left(\varepsilon_{12} + \frac{i}{\tau}\right)^2 + \left|V_{12}\right|^2}.$$

Рассмотрим случай $|V_{12}| \ll 1/\tau$. Тогда из (2.82)

$$\omega^{(1)} \approx \varepsilon_{12} + \frac{i}{\tau}, \quad \omega^{(2)} \approx \frac{V_{12}^2}{\varepsilon_{12}^2 + \frac{1}{\tau^2}}\frac{t}{\tau}.$$

Следовательно, состояние $2s_{1/2}$ имеет в этом случае очень большое время жизни $\sim 1/\left|V_{12}\right|^2\tau$.

Рассмотрим теперь противоположный предельный случай, когда наложенное поле столь велико, что $|V_{12}| \gg 1/\tau$. Тогда

$$\omega^{(1.2)} \approx \frac{1}{2}\left(\varepsilon_{12} + \frac{i}{\tau}\right) \pm \left|V_{12}\right| \pm \frac{1}{8\left|V_{12}\right|}\left(\varepsilon_{12} + \frac{i}{\tau}\right)^2$$

и время затухания C_1 становится равным по порядку величины времени жизни дипольного состояния τ.

Итак, время жизни состояния $2s_{1/2}$ атома водорода чрезвычайно сильно (на девять порядков) уменьшается при наложении электрического поля порядка $\mathscr{E} \sim \frac{1}{x_{12}\tau} \sim \frac{1}{\tau} \sim c^{-3} \sim \frac{10^9}{c^3} - B \sim 500B$.

6.3.7 Other Perturbation Theories: Overview

(нужно будет - поразбираю некоторые! пока для меня это просто есть и все, пока не работал с ними почти никак или вообще никак.)

On Schrieffer–Wolff transformation (????)

(так оказывается можно делать, см. вики мб. пока ничего не знаю.)

Суть

In quantum mechanics, the Schrieffer-Wolff transformation is a unitary transformation used to perturbatively diagonalize the system Hamiltonian to first order in the interaction. As such, the Schrieffer-Wolff transformation is an operator version of second-order perturbation theory. The Schrieffer-Wolff transformation is often used to project out the high energy excitations of a given quantum many-body Hamiltonian in order to obtain an effective low energy model.[1] The Schrieffer-Wolff transformation thus provides a controlled perturbative way to study the strong coupling regime of quantum-many body Hamiltonians. Although commonly attributed to the paper in which the Kondo model was obtained from the Anderson impurity model by J.R. Schrieffer and P.A. Wolff., [2] Joaquin Mazdak Luttinger and Walter Kohn used this method in an earlier work about non-periodic $k \cdot p$ perturbation theory. [3] Using the Schrieffer-Wolff transformation, the high energy charge excitations present in Anderson impurity model are projected out and a low energy effective Hamiltonian is obtained which has only virtual charge fluctuations. For the Anderson impurity model case, the Schrieffer-Wolff transformation showed that the Kondo model lies in the strong coupling regime of the Anderson impurity model.

см мб то, что гуглится: Bravyi, Sergey, DiVincenzo, David P, см. сп. літературы.

Derivation

Consider a quantum system evolving under the time-independent Hamiltonian operator H of the form:

$$H = H_0 + V$$

where H_0 is a Hamiltonian with known eigenstates $|m\rangle$ and corresponding eigenvalues E_m, and where V is a small perturbation. Moreover, it is assumed without loss of generality that V is purely off-diagonal in the eigenbasis of H_0, i.e., $\langle m|V|m\rangle = 0$ for all m. Indeed, this situation can always be arranged by absorbing the diagonal elements of V into H_0, thus modifying its eigenvalues to $E'_m = E_m + \langle m|V|m\rangle$. The Schrieffer-Wolff transformation is a unitary transformation which expresses the Hamiltonian in a basis (the "dressed" basis) where it is diagonal to first order in the perturbation V. This unitary transformation is conventionally written as:

$$H' = e^S H e^{-S}$$

When V is small, the generator S of the transformation will likewise be small. The transformation can then be expanded in S using the BakerCampbell-Haussdorf formula

$$H' = H + [S, H] + \frac{1}{2}[S, [S, H]] + \ldots$$

Here, $[A, B]$ is the commutator between operators A and B. In terms of H_0 and V, the transformation becomes

$$H' = H_0 + V + [S, H_0] + [S, V] + \frac{1}{2}[S, [S, H_0]] + \frac{1}{2}[S, [S, V]] + \ldots$$

The Hamiltonian can be made diagonal to first order in V by choosing the generator S such that

$$V + [S, H_0] = 0$$

This equation always has a definite solution under the assumption that V is off-diagonal in the eigenbasis of H_0. Substituting this choice in the previous transformation yields:

$$H' = H_0 + \frac{1}{2}[S, V] + O\left(V^3\right)$$

Overview of applications of Schrieffer–Wolff transformation (????)

(?? in condensed matter, in SC. but I'll learn it later)

k·p perturbation theory (??)

(см. вики)

In solid-state physics, the k·p perturbation theory is an approximated semi-empirical approach for calculating the band structure (particularly effective mass) and optical properties of crystalline solids.[1][2][3] It is pronounced "k dot p", and is also called the k·p method. This theory has been applied specifically in the framework of the Luttinger–Kohn model (after Joaquin Mazdak Luttinger and Walter Kohn), and of the Kane model (after Evan O. Kane).

Main ideas

(????)

Overview of applications

(????)

M∅ller–Plesset perturbation theory

Main ideas

(????)

Overview of applications

(????)

6.3.8 Other Properties of Perturbation Theories

Let's discuss features of perturbation theories, which are 100% not needed to know for basic understanding.

Двойные переходы в рамках теории возмущений (?????)

Допустим, система находится на одном уровне. Она может перейти на второй в рамках 1го порядка ТВ. Дальше с него в рамках 2го порядка она может вернуться на 1-й. Может ли эта вероятность перехода во 2м порядке повлиять на суммарную вероятность остаться в 1м состоянии? Или же вероятность остаться во 2м порядке такая же, как и без учета этого перехода?

(не знаю, мб нет, потому что квантмех так устроен, что у нас только 1 переход между измерениями. Это тот вопрос, который нужно задать настоящим профессионалам.)

Connection of PT method in quantum and classical mechanics

(?? first, I'll write it in classical mechanics)

Connection of PT method in quantum mechanics and in differential equations

(PT is also a typical method for diff eq. so, is it the same as here??)

6.4 Harmonic Oscillator: Basics

Изучим подробно гармонический осциллятор.

6.4.1 Quantization of a Harmonic Oscillator

мотивация

гармонический осциллятор - одна из самых распространенных моделей квантовой механики.

На основе ее и поля квантуются, и показывается, как операторы рождения и уничтожения вводятся (и что еще?) и что только ни делается.

Разберем здесь эту модель.

вкратце теория

Выпишем тезисно все выводы, которые дальше будем получать.

В квантовой механике координатам a и a^* соответствует какая-то пара операторов $\hat{a}$ и $\hat{a}^\dagger$. Константу C удобно выбрать так, чтобы операторы получились безразмерными, что соответствует следующему выбору:

$$\begin{cases} \hat{a} = \frac{1}{\sqrt{2}}(\hat{X} + i\hat{P}) = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2\hbar m\omega}}\hat{p} \\ \hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{X} - i\hat{P}) = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2\hbar m\omega}}\hat{p} \end{cases}, \quad \begin{cases} \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right) \\ \hat{p} = -i\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a} - \hat{a}^\dagger\right) \end{cases}$$

(выбор фазы остаётся произвольным - скажем, операторы $\hat{a}e^{i\varphi}$ и $\hat{a}^\dagger e^{-i\varphi}$ ничем не хуже). Наконец, можно выразить через эти операторы также и гамильтониан.

Тривиальной подстановкой, получаем:

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$$

рассмотрим частицу в потенциале $U = m\omega^2 x^2/2$

для него есть функция Гаусса

$$\psi_0(x) = \sqrt[4]{\frac{m\omega}{\pi\hbar}}e^{-\frac{X^2}{2(\hbar/nm\omega)}}$$

волновая функция:

$$\psi_n(x) = e^{-\frac{X^2}{2(\hbar/nm\omega)}}H_n(x)$$

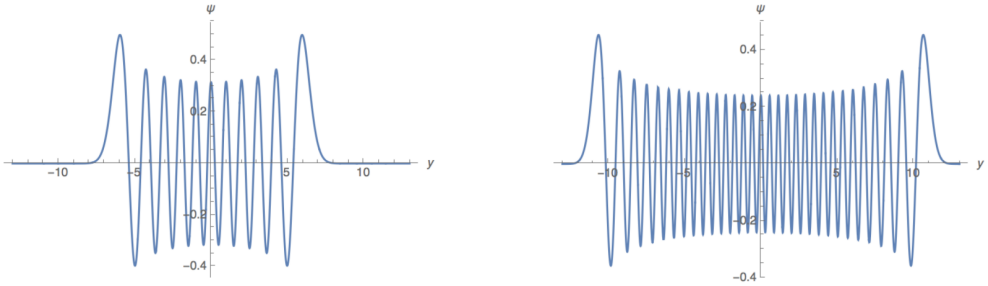


Figure 6.2: Состояния 20-го и 60-го номера по Тонгу

The 3d Harmonic Oscillator

(пока по Тонгу)

The harmonic oscillator provides a particularly simple example of the 3d Schrödinger equation because we can solve it in either Cartesian or polar coordinates. In Cartesian coordinates, the Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{1}{2}m\omega^2\left(x^2 + y^2 + z^2\right)$$

We see that the Hamiltonian just decomposes into three copies of the 1d harmonic oscillator: one for each direction. This means that we can just read off the energy spectrum from our earlier result (2.29). The spectrum of the 3d harmonic oscillator is given by

$$E = \hbar\omega\left(\frac{3}{2} + N\right)$$

where

$$N = n_1 + n_2 + n_3 \quad , n_i = 0, 1, 2, ...$$

All of the subtleties lie in the degeneracy of the spectrum. The ground state has energy $E = \frac{3}{2}\hbar\omega$ and is unique. But there are three excited states with energy $E = \frac{5}{2}\hbar\omega$ associated to exciting the harmonic oscillator in the x, y or z direction. There are then 6 states with energy $E = \frac{7}{2}\hbar\omega$, because we could excite one oscillator twice or two oscillators once each. In general, the degeneracy of the N^{th} level is $\frac{1}{2}(N+1)(N+2)$. How does this look in polar coordinates? It's best to work with the form of the Schrödinger equation (4.13) which is now

$$-\frac{\hbar^2}{2mr^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left(\frac{1}{2}m\omega^2 r^2 + \frac{l(l+1)\hbar^2}{2mr^2}\right)R = ER$$

We're now awash with various constants and life will be easier if we can get rid of a few. We make the same scaling (2.22) that we used for the 1 d oscillator,

$$y = \sqrt{\frac{m\omega}{\hbar}}r \quad \text{and} \quad \tilde{E} = \frac{2E}{\hbar\omega}$$

The Schrödinger equation then becomes

$$\frac{1}{y^2}\frac{d}{dy}\left(y^2\frac{dR}{dy}\right) - \left(y^2 + \frac{l(l+1)}{y^2}\right)R = -\tilde{E}\psi$$

We're going to solve it using the same kind of polynomial expansion that we used for the 1 d harmonic oscillator. First, look at the large distance $y \to \infty$ behaviour. Here the dominant terms are

$$\frac{d^2R}{dy^2} - y^2R \approx 0 \quad \Longrightarrow \quad R \approx e^{-y^2/2} \quad \text{as } y \to \infty$$

Next, look at the behaviour near the origin $y \ll 1$. Here the dominant terms in the equation are

$$\frac{d^2R}{dy^2} + \frac{2}{y}\frac{dR}{dy} - \frac{l(l+1)}{y^2}R \approx 0 \quad \text{for } y \ll 1$$

If we make the power-law ansatz $R \sim y^\alpha$, we find

$$\alpha(\alpha-1) + 2\alpha - l(l+1) = 0 \quad \Longrightarrow \quad R \sim y^l \text{ as } y \to 0$$

Here we've discarded the second solution $\alpha = -(l+1)$ on the grounds that the resulting wavefunction diverges at the origin. Putting this together, our ansatz for the general solution is

$$R(y) = y^l h(y) e^{-y^2/2}$$

where we take

$$h(y) = \sum_{k=0}^{\infty} a_k y^k$$

At this stage we've got a little bit of algebra to do, plugging our ansatz into the Schrödinger equation (4.16). Once the dust settles, you'll find the result

$$\sum_{k=0}^{\infty} a_k \left(k(2l+k+1)y^{l+k-2} + (\bar{E} - (2l+2k+3))y^{l+k} \right) = 0$$

We start our recursion relation by setting

$$a_0 = 1$$

This is just the statement that the small y behaviour is indeed $R \sim y^l$ rather than some higher power. Now note that the first term in our equation will have term proportional to $a_1 y^{l-1}$. But there's nothing to cancel this in the second term. This means that we must set

$$a_1 = 0$$

As we'll see, our recursion relation will then set $a_k = 0$ for all odd k. To find this recursion relation, we shift the summation variable $k \to k+2$ in the first term in (4.18) so that all terms have the same power of y^{l+k},

$$\left[\sum_{k=0}^{\infty} a_{k+2}(k+2)(2l+k+3) + \sum_{k=0}^{\infty} a_k(\bar{E} - (2l+2k+3)) \right] y^{l+k} = 0$$

For this to hold for all y, we must have the following recursion relation

$$a_{k+2} = \frac{\bar{E} - (2l+2k+3)}{(k+2)(2l+k+3)} a_k$$

At this stage, the argument is the same as we used for the 1d harmonic oscillator. If the recursion relation fails to terminate then $a_{k+2} \to 2a_k/k$ for large k, but that's bad: it messes up the $e^{-y^2/2}$ behaviour at large y and turns it into a non-normalisable $e^{+y^2/2}$ behaviour. This means that we must find solutions where the recursion relation terminates. This immediately allows us to read off the energy. If we are to have $a_{2q+2} = 0$ (recall that all a_k for odd k already vanish) then the energy of the state must be

$$E = \hbar\omega \left(\frac{3}{2} + l + 2q \right) \quad l, q = 0, 1, 2, ...$$

Let's compare this to our Cartesian result (4.15). Clearly they agree, but the extra work we did in polar coordinates brings more information: it tells us how the energy depends on the total angular momentum l. In particular, the lowest energy state with angular momentum l has $E = \hbar\omega\left(\frac{3}{2} + l\right)$.

Вырождение пространственного осциллятора (!?!?)

We also have a better understanding of the degeneracy of states. When N is even, the states with energy $E = \hbar\omega\left(\frac{1}{2} + N\right)$ comprise of all even angular momentum states $l = 0, 2, 4, ..., N$. Since there are $2l + 1$ states (4.14) associated to each angular momentum l, the total number of states at level N must be

Total Degeneracy $= \sum_{k=0}^{N/2} 4k + 1 = N\left(\frac{N}{2} + 1\right) + \frac{N}{2} + 1 = \frac{1}{2}(N + 1)(N + 2)$ which agrees with the count from the Cartesian calculation. Similarly, when N is odd the states at energy $E = \hbar\omega\left(\frac{1}{2} + N\right)$ comprise of all odd angular momentum states $l = 1, 3, 5, ..., N$: again, the total count is $\frac{1}{2}(N + 1)(N + 2)$.

Вырождение трехмерного осциллятора

(типичная заготовка, важно разбираться, потом напишу нормально. пока достаточно неплохо в интернете написано.)

Частица массы m_0 движется в трехмерном потенциальном поле

$$U(x, y, z) = \frac{k}{2}\left(x^2 + y^2 + z^2\right),$$

Решение: Поскольку движение частицы вдоль осей x, y и z происходит независимо, то будем искать волновую функцию в виде произведения

$$\psi_2(y) \cdot \psi_3(z) \cdot \frac{d^2\psi_1(x)}{dx^2} + \psi_1(x) \cdot \psi_3(z)\frac{d^2\psi_2(y)}{dy^2} + \psi_1(x) \cdot \psi_2(y) \cdot \frac{d^2\psi_3(z)}{dz^2}$$

$$+\frac{2m_0}{\hbar^2}[E - U(x, y, z)]\psi_1(x) \cdot \psi_2(y) \cdot \psi_3(z) = 0.$$

Разделив это уравнение на $\psi(x, y, z)$ и используя данный в условии задачи вид зависимости $U(x, y, z)$, приходим к соотношению

$$\left[\frac{1}{\psi_1(x)} \cdot \frac{d^2\psi_1(x)}{dx^2} - \frac{2m_0}{\hbar^2} \cdot \frac{kx^2}{2}\right] + \left[\frac{1}{\psi_2(y)} \cdot \frac{d^2\psi_2(y)}{dy^2} - \frac{2m_0}{\hbar^2} \cdot \frac{ky^2}{2}\right] +$$
$$+ \left[\frac{1}{\psi_3(z)} \cdot \frac{d^2\psi_3(z)}{dz^2} - \frac{2m_0}{\hbar^2} \cdot \frac{kz^2}{2}\right] = -\frac{2m_0}{\hbar^2}E.$$

функкцей только координаты Z. Поскольку их сумма равна постоянной величине, то каждое из этих слагаемых также должно равняться постоянной величине

$$\frac{1}{\psi_1(x)} \cdot \frac{d^2\psi_1(x)}{dx^2} - \frac{2m_0}{\hbar^2} \cdot \frac{kx^2}{2} = -\frac{2m_0}{\hbar^2}E_1$$
$$\frac{1}{\psi_2(y)} \cdot \frac{d^2\psi_2(y)}{dy^2} - \frac{2m_0}{\hbar^2} \cdot \frac{ky^2}{2} = -\frac{2m_0}{\hbar^2}E_2$$

нам уже известны (см. (4.81), (4.83)).

n_2un_3

$$\psi_{x_1,x_2,x_3}(x, y, z) = \psi_{x_1}(x) \cdot \psi_{x_i}(y) \cdot \psi_{x_3}(z),$$
$$n_1, n_2, n_3 = 0, 1, 2, 3, ...$$

Для энераии трехмерного гармонического осциллятора получаем следующее выражение

$$E_n = \hbar\omega_0\left(n + \frac{3}{2}\right)$$

где $n = n_1 + n_2 + n_3, n = 0, 1, 2, 3, ...$

Найдем кратность вырождения n - го энергетического уровня трехмерного гармонического осциллятора. Дпя заданного значения n кратность вырождения уровня равна числу возможных перестановок трех чисел n_1. n_2 и n_3, сумма которых раена n. Найдем сначала число перестановок при фиксированном значении n_1. Оно, как легко видеть, равно числу возможных значений n_2 (или, что то же самое, n_3). Число n_2 при заданном n_1 может меняться в пределах от одо $(n - n_1)$, т.е. принимает $n - n_1 + 1$ значение. Следовательно, число перестановок при фиксированном n_1 равно $n - n_1 + 1$. Суммируя это выражение по n_1, находим кратность вырождения n-го уровня K_n

$$K_n = \sum_{n_1=0}^{n} (n - n_1 + 1) = \frac{(n+1)(n+2)}{2}.$$

Основное состояние трехмерного гармонического осциллятора ($n = 0$) оказывается невырожденным, $K_0 = 1$. Первое возбужденное состояние ($n = 1$) имеет кратность вырождения $K_1 = 3$, ему соответствуют тройки квантовых чисел (100), (010), (001)

(ну и поэтому на осциллятор есть задачи с применением вырожденной теории возмущений.)

точное решение

(птф, пока просто скрины)

Поучительно будет рассмотреть вырожденную гипергеометрическую функцию на примере простого гармонического осциллятора - частицы в потенциале $U(x) = \frac{m\omega^2 x^2}{2}$.

Поскольку потенциальная энергия $U(x \to \pm\infty) \to \infty$, то в этом потенциале нет непрерывного спектра, а только дискретный.

Переходя к безразмерной координате $y = x\sqrt{\frac{m\omega}{\hbar}}$ и вводя безразмерную энергию согласно $E = \hbar\omega\left(\epsilon + \frac{1}{2}\right)$, мы получаем уравнение Шрёдингера в виде:

$$\psi''(y) + \left(2\epsilon + 1 - y^2\right)\psi(y) = 0$$

Сделаем замену координат $z = y^2 \to y = \sqrt{z}$:

$$\frac{d\psi}{dy} = 2\sqrt{z}\frac{d\psi}{dz}, \quad \frac{d^2\psi}{dy^2} = 2\sqrt{z}\frac{d}{dz}\left(2\sqrt{z}\frac{d\psi}{dz}\right) = 4z\psi''(z) + 2\psi'(z)$$

$$4z\psi''(z) + 2\psi'(z) + (2\epsilon + 1 - z)\psi(z) = 0$$

Мы получили уравнение с линейными коэффициентами, значит, его можно привести к ${}_1F_1$.

Стандартный способ такой процедуры - это выделение асимптотик.

В частности, при $z \to \infty$, асимптотический вид уравнения выглядит как

$$4z\psi''(z) - z\psi(z) = 0 \to \psi(z) \approx e^{-z/2}.$$

Поэтому мы сделаем подстановку $\psi(z) = \chi(z)e^{-z/2}$; получаем:

$$z\chi''(z) + \left(\frac{1}{2} - z\right)\chi'(z) + \frac{\epsilon}{2}\chi(z) = 0$$

В нашем конкретном случае $b = \frac{1}{2}, a = -\frac{\epsilon}{2}$, и поэтому общее решение уравнения записывается следующим образом:

$$\chi(z) = C_1 \cdot {}_1F_1\left(-\frac{\epsilon}{2}; \frac{1}{2}; z\right) + C_2\sqrt{z} \cdot {}_1F_1\left(-\frac{\epsilon - 1}{2}; \frac{3}{2}; z\right)$$

В общем случае ${}_1F_1 \sim e^z$, что соответствует экспоненциально растущей волновой функции и нас не устраивает, поэтому ряд должен обрываться.

Имеются две альтернативы: что, конечно, исчерпывает все решения задачи о простом гармоническом осцилляторе.

Для справки приведём связь написанных тут гипергеометрических функций с полиномами Эрмита и нормированными волновыми функциями:

(????)

6.4.2 Quantization of a Harmonic Oscillator with Features

возбуждения под действием $-F\hat{x}c^{-t^2}$

Рассмотрим задачу об возбуждении гармонического осциллятора под действием силы, которая действует в течении конечного времени:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2} - F\hat{x}c^{-t^2/\tau^2}$$

Допустим, при $t \to -\infty$ мы находились в основном состоянии осциллятора $|i\rangle = |0\rangle$;

ищем мы вероятность перехода в первое и второе возбуждённые состояния.

Определим, какие матричные элементы возмущения вообще отличны от нуля.

Используя лестничные операторы, мы видим, что отличны от нуля только переходы между соседними уровнями:

$$V_{nm}(t) = -Fe^{-t^2/\tau^2}\langle n|\hat{x}|m\rangle = -\frac{Fe^{-t^2/\tau^2}}{\sqrt{2m\omega}} \cdot \begin{cases} \sqrt{n}, & m = n-1 \\ \sqrt{n+1}, & m = n+1 \end{cases}$$

В частности, в первом порядке теории возмущений переход происходит только в первое возбуждённое состояние, разница энергий которых равна $\omega_{10} = \omega$:

$$w_{0\to 1} = \left| -\frac{F}{\sqrt{2m\omega}} \int\limits_{-\infty}^{\infty} e^{-t^2/\tau^2} e^{i\omega t} dt \right|^2 = \frac{\pi F^2 \tau^2}{2m\omega} e^{-\omega^2\tau^2/2}$$

Требуя малость поправки, мы приходим к выводу, что теория возмущений работает по параметру $F^2\tau^2/m\omega \ll 1$ либо $\omega\tau \gg 1$ Чтобы найти вероятность перехода во второе возбуждённое состояние, первого порядка теории возмущений недостаточно, и нужно решить уравнение (5.32) точнее.

Во втором приближении, получаем:

$$\partial_t \psi_2^{(2)}(t) = -i \int\limits_{-\infty}^{t} d\tau_1 V_{21}^{(I)}(\tau_1)\, \psi_1^{(1)}(\tau_1) = (-i)^2 \int\limits_{-\infty}^{t} d\tau_1 V_{21}^{(I)}(\tau_1) \int\limits_{-\infty}^{\tau_1} d\tau_2 V_{10}^{(I)}(\tau_2)$$

а значит, искомая вероятность равна:

$$w_{0\to 2} = \left| \int\limits_{-\infty}^{\infty} d\tau_1 V_{21}(\tau_1)\, e^{i\omega\tau_1} \int\limits_{-\infty}^{\tau_1} d\tau_2 V_{10}(\tau_2)\, e^{i\omega\tau_2} \right|^2 =$$

$$= \frac{2F^4}{(2m\omega)^2} \left| \int\limits_{-\infty}^{\infty} d\tau_1 e^{-\tau_1^2/\tau^2 + i\omega\tau_1} \int\limits_{-\infty}^{\tau_1} d\tau_2 e^{-\tau_2^2/\tau^2 + i\omega\tau_2} \right|^2$$

Можно заметить, что стоящий тут интеграл равен половине такого же интеграла, но с бесконечными пределами $\int\limits_{-\infty}^{\infty} d\tau_1 \int\limits_{-\infty}^{\infty} d\tau_2$ благодаря чему мы можем сразу выписать для него результат:

$$w_{0\to 2} = \frac{\pi^2 F^4 \tau^4}{8m^2\omega^2} e^{-\omega^2\tau^2}$$

Полученный результат оказался параметрически меньше $w_{0\to 1}$, поскольку он связан со вторым порядком теории возмущений.

Математические указания для работы с осциллятором (!?!?)

(это важно, без этого ничего не сделаешь, упершись только в математику.)

применение модели гармонического осциллятора

(укажу потом????)

6.4.3 Harmonic Oscillator by Takhtajan

Простейшая классическая система с одной степенью свободы, за исключением свободной частицы, - это гармонический осциллятор. Он описывается фазовым пространством $\mathbb{R}^2$ с каноническими координатами p, q и функцией Гамильтона

$$H_{\mathrm{c}}(p,q) = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}$$

(см. разделы 1.1.5 и 1.1.7 главы 1). Уравнения Гамильтона

$$\dot{p} = \{H_{\mathrm{c}}, p\} = -m\omega^2 q, \quad \dot{q} = \{H_{\mathrm{c}}, q\} = \frac{p}{m}$$

с начальными условиями p_0, q_0 легко решаются:

$$p(t) = p_0 \cos\omega t - m\omega q_0 \sin\omega t$$
$$q(t) = q_0 \cos\omega t + \frac{1}{m\omega} p_0 \sin\omega t$$

и описывают гармоническое движение. Как и в разделе 1.2.6 главы 1, удобно ввести комплексные координаты на фазовом пространстве $\mathbb{R}^2 \simeq \mathbb{C}$,

$$z = \frac{1}{\sqrt{2\omega}}(\omega q + ip), \quad \bar{z} = \frac{1}{\sqrt{2\omega}}(\omega q - ip)$$

Имеем

$$\{z, \bar{z}\} = \frac{i}{m}, \quad H_{\mathrm{c}}(z,\bar{z}) = m\omega|z|^2$$

так что уравнения Гамильтона разделяются:

$$\dot{z} = \{H_{\mathrm{c}}, z\} = -i\omega z, \quad \dot{\bar{z}} = \{H_{\mathrm{c}}, \bar{z}\} = i\omega\bar{z}$$

и тривиально решаются:

$$z(t) = e^{-i\omega t} z_0, \quad \bar{z} = e^{i\omega t}\bar{z}_0$$

Здесь

$$z_0 = \frac{1}{\sqrt{2\omega}}\left(\omega q_0 + ip_0\right), \quad \bar{z}_0 = \frac{1}{\sqrt{2\omega}}\left(\omega q_0 - ip_0\right)$$

Для квантовой системы соответствующий оператор Гамильтона - это

$$H = \frac{P^2}{2m} + \frac{m\omega^2 Q^2}{2}$$

и в координатном представлении $\mathscr{H} = L^2(\mathbb{R}, dq)$ - это оператор Шрёдингера с квадратичным потенциалом,

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{m\omega^2 q^2}{2}$$

Квантовый гармонический осциллятор - простейшая нетривиальная квантовая система, за исключением свободной частицы, у которой явно решается уравнение Шрёдингера. Он появляется во всех задачах, связанных с квантованными колебаниями, то есть в молекулярных и кристаллических вибрациях. Точное решение гармонического осциллятора, описываемое ниже, обладает замечательными [24] алгебраическими и аналитическими свойствами.

На время положим $m = 1$ и рассмотрим операторы

$$a = \frac{1}{\sqrt{2\omega\hbar}}(\omega Q + iP), \quad a^* = \frac{1}{\sqrt{2\omega\hbar}}(\omega Q - iP)$$

являющиеся квантовыми аналогами комплексных координат (2.30). Операторы a и a^* определены на $W^{1,2}(\mathbb{R}) \cap \widehat{W^{1,2}}(\mathbb{R})$, где $\widehat{W}^{1,2}(\mathbb{R}) = \mathscr{F}\left(W^{1,2}(\mathbb{R})\right)$, и легко показать, что a^* - сопряженный оператор к a и $a^{**} = a$, так что a - замкнутый оператор. Из коммутационных соотношений Гейзенберга (2.2) мы получаем каноническое коммутачионное соотношение

$$[a, a^*] = I$$

на $W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$. Действительно

$$aa^* = \frac{P^2 + \omega^2 Q^2}{2\omega\hbar} + \frac{i\omega}{2\omega\hbar}[P, Q] = \frac{P^2 + \omega^2 Q^2}{2\omega\hbar} + \frac{1}{2}I,$$

и

$$a^*a = \frac{P^2 + \omega^2 Q^2}{2\omega\hbar} - \frac{i\omega}{2\omega\hbar}[P, Q] = \frac{P^2 + \omega^2 Q^2}{2\omega\hbar} - \frac{1}{2}I$$

так что (2.34) выполняется на $W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$, где $\widehat{W}^{2,2}(\mathbb{R}) = \mathscr{F}\left(W^{2,2}(\mathbb{R})\right)$, и

$$H = \omega\hbar\left(a^*a + \frac{1}{2}I\right) = \omega\hbar\left(aa^* - \frac{1}{2}I\right).$$

В частности, из критерия фон Неймана следует, что оператор Гамильтона H самосопряжен.

[24] Алгебраическая структура точного решения гармонического осциллятора играет фундаментальную роль в квантовой электродинамике и вообще в квантовой теории поля. Операторы a, a^* и $N = a^*a$ удовлетворяют коммутационным соотношениям

$$[N, a] = -a, \quad [N, a^*] = a^*, \quad [a, a^*] = I.$$

Эти коммутационные соотношения соответствуют неприводимому унитарному представлению четырехмерной разрешимой алгебры Ли $\tilde{\mathfrak{h}}$, ассоциированной с алгеброй

Гейзенберга $\mathfrak{h} = \mathfrak{h}_1$, введенной в разделе 2.2.1. А именно: $\tilde{h}$ - алгебра Ли с образующими e, f, h, и c, где e, f, c удовлетворяют соотношениям алгебры Гейзенберга $\mathfrak{h}$ и

$$[h, e] = -f, \quad [h, f] = \omega^2 e, \quad [h, c] = 0.$$

Неприводимое интегрируемое представление ρ алгебры Гейзенберга $\mathfrak{h}$ (см. (2.9) в разделе 2.2.1) продолжается до унитарного представления алгебры Ли $\tilde{\mathfrak{h}}$, если положить

$$\rho(h) = -i\omega N = \frac{P^2 + \omega^2 Q^2}{2i\hbar} + \frac{i\omega}{2} I$$

ЗАМЕЧАНИЕ. В инвариантных терминах алгебра Ли $\tilde{\mathfrak{h}}$ - одномерное праве расширение алгебры Гейзенберга $\mathfrak{h}$,

$$0 \to \mathfrak{h} \to \tilde{\mathfrak{h}} \to \mathbb{R} \to 0$$

Оно определяется $\mathfrak{h}$-значным 1-коциклом $r \in Z^1(\mathfrak{h}, \mathfrak{h})$ на алгебре Ли - дифференциальным оператором на $\mathfrak{h}$, задаваемым на образующих формулой

$$r(e) = f, \quad r(f) = -\omega^2 e, \quad r(c) = 0$$

Конкретно, если $h \in \tilde{\mathfrak{h}}$ таково, что $\bar{h} = 1 \in \mathbb{R}$ при проекции $\tilde{\mathfrak{h}} \to \mathbb{R}$, то, отождествляя элементы $\mathfrak{h}$ с их образами при вложении $\mathfrak{h} \hookrightarrow \tilde{\mathfrak{h}}$, имеем

$$[x + \alpha h, y + \beta h] = [x, y] - \alpha r(y) + \beta r(y), \quad x, y \in \mathfrak{h}.$$

Как раз благодаря этой Ли-алгебраической структуре коммутационных соотношений (2.35), уравнения движения Гейзенберга для гармонического осциллятора точно решаются. А именно: мы имеем

$$\dot{a} = \{H, a\}_\hbar = -i\omega a, \quad \dot{a}^* = \{H, a^*\}_\hbar = i\omega a^*$$

так что

$$a(t) = e^{-i\omega t} a_0, \quad a^*(t) = e^{i\omega t} a_0^*$$

Сравнивая с (2.32), видим, что решения классических и квантовых уравнений движения гармонического осциллятора имеют один и тот же вид! Далее, используя коммутационные соотношения (2.35) и положительность оператора N, мы решим задачу на собственные значения гамильтониана H гармонического осциллятора, в явном виде определив его уровни энергии и соответствующие собственные вектора. Мы докажем, что собственные вектора образуют полную систему векторов в $\mathscr{H}$, так что спектр гамильтониана H является точечным. Это квантово-механический аналог того факта, что классическое движение гармонического осциллятора всегда финитно.

Алгебраическая часть точного решения состоит из следующего фундаментального результата.

Предложение 2.2.

Допустим, что существует ненулевое $\psi \in D(a^n) \cap \cap D((a^*)^n), n = 1, 2, ...$, такое, что

$$H\psi = \lambda\psi$$

Тогда выполняются следующие утверждения.

(i) Существует $\psi_0 \in \mathscr{H}, \|\psi_0\| = 1$, такое, что

$$H\psi_0 = \frac{1}{2}\hbar\omega\psi_0$$

(ii) Векторы

$$\psi_n = \frac{(a^*)^n}{\sqrt{n!}}\psi_0 \in \mathscr{H}, \quad n = 0, 1, 2, ...,$$

ортонормальные собственные векторы H с собственными значениями $\hbar\omega\left(n + \frac{1}{2}\right)$

$$H\psi_n = \hbar\omega\left(n + \frac{1}{2}\right)\psi_n$$

(iii) Ограничение оператора H на гильбертово пространство $\mathscr{H}_0$ - замкнутое подпространство $\mathscr{H}$, натянутое на ортонормальное множество $\{\psi_n\}_{n=0}^{\infty}$ - самосопряжено в существенном.

ДОКАЗАТЕЛЬСТВО.

Переписывая коммутационные соотношения (2.35) как

$$Na = a(N - I) \quad \text{и} \quad Na^* = a^*(N + I)$$

и положив $\lambda = \hbar\omega\left(\mu + \frac{1}{2}\right)$, получаем для всех $n \geqslant 0$

$$Na^n\psi = (\mu - n)a^n\psi \quad \text{и} \quad N\left(a^*\right)^n\psi = (\mu + n)\left(a^*\right)^n\psi$$

Поскольку $N \geqslant 0$ на $D(N)$, из первого уравнения в (2.36) следует, что существует $n_0 \geqslant 0$, такое, что $a^{n_0}\psi \neq 0$, но $a^{n_0+1}\psi = 0$. Положив $\psi_0 = \frac{a^{n_0}\psi}{\|a^{n_0}\psi\|} \in \mathscr{H}$, получаем

$$a\psi_0 = 0 \quad \text{и} \quad N\psi_0 = 0$$

Поскольку $H = \hbar\omega\left(N + \frac{1}{2}I\right)$, это доказывает часть (i). Для доказательства части (ii) воспользуемся коммутационными соотношениями

$$[a, (a^*)^n] = n\,(a^*)^{n-1}$$

которые следуют из (2.34) и правила Лейбница. Используя (2.37)- (2.38), получаем

$$a^*\psi_n = \sqrt{n+1}\psi_{n+1}, \quad a\psi_n = \sqrt{n}\psi_{n-1},$$

так что

$$\begin{aligned}\|\psi_n\|^2 &= \frac{1}{\sqrt{n}}\left(a^*\psi_{n-1}, \psi_n\right) = \\ &= \frac{1}{\sqrt{n}}\left(\psi_{n-1}, a\psi_n\right) = \|\psi_{n-1}\|^2 = ... = \|\psi_0\|^2 = 1.\end{aligned}$$

Из второго уравнения в (2.36) следует, что $N\psi_n = n\psi_n$, поэтому ψ_n - нормализованные собственные векторы H с собственными значениями $\hbar\omega\left(n + \frac{1}{2}\right)$. Собственные векторы ψ_n ортогональны, поскольку соответствующие собственные значения различны, а оператор H симметрический. Наконец, часть (iii) мгновенно следует из того факта, что, согласно части (ii), подпространства $\mathrm{Im}(H \pm iI)|_{\mathscr{H}_0}$ плотны в $\mathscr{H}_0$, что является критерием самосопряженности в существенном.

ЗАМЕЧАНИЕ. Поскольку координатное представление коммутационных соотношений Гейзенберга неприводимо, заманчиво заключить, используя предложение

2.2, что $\mathscr{H}_0 = \mathscr{H}$. А именно: из построения следует, что линейная оболочка векторов ψ_n - плотное подпространство в $\mathscr{H}_0$ - инвариантна относительно операторов P и Q. Однако из этого не следует сразу, что оператор Π_0 проекции на подпространство $\mathscr{H}_0$ коммутирует с самосопряженными операторами P и Q в смысле определения в разделе 2.1.1.

Используя координатное представление, можно мгновенно показать существование вектора ψ_0 в предложении 2.2 и доказать, что $\mathscr{H}_0 = \mathscr{H}$. Действительно, уравнение $a\psi_0 = 0$ превращается в линейное дифференциальное уравнение первого порядка:

$$\left(\hbar\frac{d}{dq} + \omega q\right)\psi_0 = 0$$

так что

$$\psi_0(q) = \sqrt[4]{\frac{\omega}{\pi\hbar}}e^{-\frac{\omega}{2\hbar}q^2}$$

и

$$\|\psi_0\|^2 = \sqrt{\frac{\omega}{\pi\hbar}}\int\limits_{-\infty}^{\infty} e^{-\frac{\omega}{\hbar}q^2}dq = 1.$$

Вектор ψ_0 называется основным состоянием гармонического осциллятора. Соответственно, собственные функции

$$\psi_n(q) = \frac{1}{\sqrt{n!}}\left(\frac{1}{\sqrt{2\omega\hbar}}\left(\omega q - \hbar\frac{d}{dq}\right)\right)^n\psi_0$$

имеют вид $P_n(q)e^{-\frac{\omega}{2\hbar}q^2}$, где $P_n(q)$ - многочлены степени n. Следующий результат показывает, что функции $\{\psi_n\}_{n=0}^{\infty}$ образуют ортонормальный базис в $L^2(\mathbb{R}, dq)$.

Лемма 2.3. Функции $q^n e^{-q^2}, n = 0, 1, 2, ...$, полны в $L^2(\mathbb{R}, dq)$.

ДОКАЗАТЕЛЬСТвО.

Пусть $f \in L^2(\mathbb{R}, dq)$ таково, что

$$\int\limits_{-\infty}^{\infty} f(q)q^n e^{-q^2}dq = 0, \quad n = 0, 1, 2, ...$$

Интеграл

$$F(z) = \int\limits_{-\infty}^{\infty} f(q)e^{iqz-q^2}dq$$

абсолютно сходится для всех $z \in \mathbb{C}$ и поэтому определяет целую функцию. Имеем

$$F^{(n)}(0) = i^n\int\limits_{-\infty}^{\infty} f(q)q^n e^{-q^2}dq = 0, \quad n = 0, 1, 2, ...$$

так что $F(z) = 0$ для всех $z \in \mathbb{C}$. Из этого следует, что функция $g(q) = f(q)e^{-q^2} \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ удовлетворяет условию $\mathscr{F}(g) = 0$, где $\mathscr{F}$ «обычное» ($\hbar = 1$) преобразование Фурье. Таким образом, мы заключаем, что $g = 0$. Многочлены P_n выражаются через классические многочлены Эрмита-Чебышева H_n, определяемые формулой

$$H_n(q) = (-1)^n e^{q^2} \frac{d^n}{dq^n} e^{-q^2}, \quad n = 0, 1, 2, ...$$

А именно: используя тождество

$$e^{\frac{q^2}{2}} \frac{d^n}{dq^n} e^{-q^2} = -\left(q - \frac{d}{dq}\right)\left[e^{\frac{q^2}{2}} \frac{d^{n-1}}{dq^{n-1}} e^{-q^2}\right] =$$
$$= ... = (-1)^n \left(q - \frac{d}{dq}\right)^n e^{-\frac{q^2}{2}}$$

получаем

$$\psi_n(q) = \sqrt[4]{\frac{\omega}{\pi\hbar}} \frac{1}{\sqrt{2^n n!}} e^{-\frac{\omega}{2\hbar}q^2} H_n\left(\sqrt{\frac{\omega}{\hbar}} q\right).$$

Подытожим полученные результаты следующим образом.

Th.

2.1. Гамильтониан

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dq^2} + \frac{m\omega^2 q^2}{2}$$

квантового гармонического осциллятора с одной степенью свободы является самосопряженным оператором в $\mathscr{H} = L^2(\mathbb{R}, dq)$ с областью определения $D(H) = W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$. Оператор H имеет чисто точечный спектр

$$H\psi_n = \lambda_n \psi_n, \quad n = 0, 1, 2, ...,$$

с собственными значениями $\lambda_n = \hbar\omega\left(n + \frac{1}{2}\right)$. Соответствующие собственные функции ψ_n образуют ортонормальный базис Н и даются формулами

$$\psi_n(q) = \sqrt[4]{\frac{m\omega}{\pi\hbar}} \frac{1}{\sqrt{2^n n!}} e^{-\frac{m\omega}{2\hbar}q^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}} q\right)$$

где $H_n(q)$ - классические многочлены Эрмита-Чебытева.

ДОКАЗАТЕЛЬСТВО.

Рассмотрим оператор H, определенный в пространстве Шварца $\mathscr{S}(\mathbb{R})$ быстро убывающих функций. Поскольку оператор H симметрический и имеет полную систему собственных векторов в $\mathscr{S}(\mathbb{R})$, подпространство $\mathrm{Im}(H \pm iI)$ плотно в $\mathscr{H}$, так что H самосопряжен в существенном. Доказательство того, что его самосопряженное замыкание (которое мы попрежнему будем обозначать как H) имеет областью определения пространство $W^{2,2}(\mathbb{R}) \cap \widehat{W}^{2,2}(\mathbb{R})$, остается читателю.

ЗАМЕЧАНИЕ. Уровни энергии гармонического осциллятора можно также получить из правила квантования Бора-Вильсона - Зоммерфельда. Действительно, соответствующая классическая орбита с энергией E - эллипс в фазовой плоскости, задаваемый уравнениями $q(t) = A\cos(\omega t + \alpha)$, $p(t) = -m\omega A \sin(\omega t + \alpha)$, где $E = \frac{1}{2}m\omega^2 A^2$ (см. раздел 1.1.5 главы 1). Таким образом,

$$\oint p dq = \iint dp \wedge dq = \pi m\omega A^2 = \frac{2\pi}{\omega} E$$

и по правилу квантования ББЗ получаются уровни энергии $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$.

ЗАмЕчАниЕ. Поскольку уровни энергии Гамильтона H эквидистантны с интервалом $\hbar\omega$, квантовый гармонический осциллятор описывает систему одинаковых «квантов» с энергией $\hbar\omega$. Основное состояние $|0\rangle = \psi_0$ в дираковских обозначениях - это вакуумное состояние, когда никаких квантов нет и вакуумная энергия равна $\frac{1}{2}\hbar\omega$, а состояния $|n\rangle = \psi_n$ состоят из n квантов с энергией $\hbar\omega\left(n+\frac{1}{2}\right)$. Согласно (2.39) оператор a^* добавляет состоянию $|n\rangle$ один квант, и он называется оператором рождения, а оператор a уничтожает в состоянии $|n\rangle$ один квант и называется оператором уничтожения.

Пример гармонического осциллятора - иллюстрация того, насколько отличается движение в квантовой механике от движения в классической механике. Классическое движение в потенциальном поле $V(q) = \frac{1}{2}m\omega^2q^2$ финитно: частица с энергией E движется в области $|\omega q| \leqslant \sqrt{\frac{2E}{m}}$, тогда как для квантовой частицы всегда есть ненулевая вероятность обнаружиться за пределами классической области. Так, для энергии $E = \frac{1}{2}\hbar\omega$ основного состояния эта вероятность равна

$$\int\limits_{|q|\geqslant\sqrt{\frac{\hbar}{m\omega}}} |\psi_0(q)|^2\,dq = \frac{2}{\sqrt{\pi}}\int\limits_1^\infty e^{-x^2}dx \simeq 0,1572992070.$$

Классический гармонический осциллятор с n степенями свободы описывается фазовым пространством $\mathbb{R}^{2n}$ с каноническими координатами $\boldsymbol{p},\boldsymbol{q}$ и функцией Гамильтона

$$H_{\mathrm{c}}(\boldsymbol{p},\boldsymbol{q}) = \frac{\boldsymbol{p}^2}{2m} + \sum_{j=1}^n \frac{m\omega_j^2q_j^2}{2}$$

где $\omega_1,...,\omega_n > 0$ (см. разделы 1.1.3 и 1.1.7 главы 1).

Соответствующий оператор Гамильтона есть

$$H = \frac{\boldsymbol{P}^2}{2m} + \sum_{j=1}^n \frac{m\omega_j^2Q_j^2}{2}$$

в координатном представлении $\mathscr{H} = L^2\left(\mathbb{R}^n, d^n\boldsymbol{q}\right)$ это оператор Шрёдингера с квадратичным потенциалом,

$$H = -\frac{\hbar^2}{2m}\Delta + \sum_{j=1}^n \frac{m\omega_j^2q_j^2}{2}$$

Гамильтониан H - самосопряженный оператор с $D(H) = W^{2,2}\left(\mathbb{R}^n\right) \cap \cap\widehat{W}^{2,2}\left(\mathbb{R}^n\right)$ с чисто точечным спектром. Соответствующие собственные функции

$$\psi_{\boldsymbol{k}}(\boldsymbol{q}) = \psi_{k_1}\left(q_1\right)...\psi_{\boldsymbol{k}_n}\left(q_n\right)$$

где $\boldsymbol{k} = (k_1,...,k_n)$ и $\psi_{k_j}\left(q_j\right)$ - это собственные функции (2.40)с$\omega = \omega_j$, образуют ортонормальный базис в $L^2\left(\mathbb{R}^n, d^n\boldsymbol{q}\right)$. Соответствующие уровни энергии даются формулами

$$\lambda_k = \hbar\omega_1\left(k_1+\frac{1}{2}\right) + ... + \hbar\omega_n\left(k_n+\frac{1}{2}\right)$$

Спектр H является простым, если и только если $\hbar\omega_1,...,\hbar\omega_n$ линейно независимы над $\mathbb{Z}$. Самый вырожденный случай $-\omega_1 = ... = \omega_n = \omega$, тогда кратность собственного значения

$$\lambda_k = \hbar\omega\sum_{j=1}^n\left(k_j+\frac{1}{2}\right)$$

это статистическая сумма $p_n(|\boldsymbol{k}|)$, т. е. число представлений целого числа $|\boldsymbol{k}| = k_1 + ... + k_n$ в виде суммы n неотрицательных целых чисел. Положив $m = 1$ и вводя операторы [25]

$$a_j = \frac{1}{\sqrt{2\omega\hbar}}\left(\omega Q_j + iP_j\right),$$
$$a_j^* = \frac{1}{\sqrt{2\omega\hbar}}\left(\omega Q_j - iP_j\right),$$

получаем канонические коммутационные соотношения операторов рождения и уничтожения для n степеней свободы:

$$[a_j, a_l] = 0, \quad \left[a_j^*, a_l^*\right] = 0, \quad [a_j, a_l^*] = \delta_{jl} I, \quad j, l = 1, ..., n,$$

обобщающие соотношение (2.34) для одной степени свободы. Операторы a_j, a_j^* и $N_j = a_j^* a_j, j = 1, ..., n$, удовлетворяют коммутационным соотношениям

$$[N_j, a_l] = -\delta_{jl} a_l, \quad [N_j, a_l^*] = \delta_{jl} a_l^*, \quad j, l = 1, ..., n.$$

В частности, оператор

$$N = \sum_{j=1}^{n} N_j = \sum_{j=1}^{n} a_j^* a_j$$

удовлетворяет соотношениям

$$[N, a_j] = -a_j, \quad \left[N, a_j^*\right] = a_j^*, \quad j = 1, ..., n,$$

и $H = \hbar\omega\left(N + \frac{n}{2} I\right)$.

Коммутационные соотношения (2.42) и (2.43) соответствуют неприводимому унитарному представлению разрешимой алгебры Ли $\tilde{\mathfrak{h}}_n$ с $3n + 1$ образующими e_j, f_j, h_j и c, где e_j, f_j, c удовлетворяют соотношениям алгебры Гейзенберга $\mathfrak{h}_n$, и

$[h_j, e_l] = -\delta_{jl} f_l, \quad [h_j, f_l] = \delta_{jl}\omega_l^2 e_l, \quad [h_j, c] = 0, \quad j, l = 1, ..., n.$

ЗАДАчА 2.9. Покажите, что $\langle H|M\rangle \geqslant \frac{1}{2}\hbar\omega$ для любого $M \in \mathscr{S}$, где H - гамильтониан гармонического осциллятора с одной степенью свободы.

[25] Здесь мы, используя стандартную евклидову метрику на $\mathbb{R}^n$, опустили индексы у Q^j. ЗАДАЧА 2.10. Пусть $q(t) = A\cos(\omega t + \alpha)$ - классическая траектория гармонического осциллятора с $m = 1$ и энергией $E = \frac{1}{2}\omega^2 A^2$, и пусть μ_α - вероятностная мера на $\mathbb{R}$, сконцентрированная в точке $q(t)$. Покажите, что выпуклая линейная комбинация мер $\mu_\alpha, 0 \leqslant \alpha \leqslant 2\pi$, является вероятностной мерой на $\mathbb{R}$ с функцией распределения $\mu(q) = \frac{\theta\left(A^2 - q^2\right)}{\pi\sqrt{A^2 - q^2}}$, где $\theta(q)$ - функция Хевисайда.

ЗАДАчА 2.11. Покажите, что когда $n \to \infty$ и $\hbar \to 0$, так что $\hbar\omega\left(n + \frac{1}{2}\right) = \frac{1}{2}\omega^2 A^2$ остается постоянным, огибающая функции распределения $|\psi_n(q)|^2$ на интервале $|q| \leqslant A$ совпадает с классической функцией распределения $\mu(q)$ из предыдущей задачи. (Указание: докажите, что существует интегральное представление

$$e^{-q^2} H_n(q) = \frac{2^{n+1}}{\sqrt{\pi}} \int_0^\infty e^{-y^2} y^n \cos\left(2qy - \frac{1}{2} n\pi\right) dy$$

и выведите асимптотическую формулу

$\psi_n(q) = \sqrt{\frac{2}{\pi}} \frac{1}{\sqrt[4]{A^2 - q^2}} \cos\left\{\frac{\omega}{2\hbar}\left(A^2 \sin^{-1}\frac{q}{A} + q\sqrt{A^2 - q^2} - \frac{1}{2}A^2\pi\right) + O(1)\right\}$

при $\hbar \to 0$ и $\hbar\left(n + \frac{1}{2}\right) = \frac{1}{2}\omega A^2, |q| < A$.)

ЗАДАЧА 2.12. Завершите доказательство теоремы 2.1.

ЗАДАЧА 2.13 (ТЕОРЕМА ОБ N-ПРЕДСТАвЛЕНИИ). Пусть $\psi \in \mathscr{S}(\mathbb{R})$. Покажите, что сходящееся в L^2 разложение $\psi = \sum_{n=0}^{\infty} c_n \psi_n$, где $c_n = (\psi, \psi_n)$, сходится в $\mathscr{S}(\mathbb{R})$. (Указание: воспользуйтесь тем, что $N\psi_n = n\psi_n$.)

ЗАДАчА 2.14. Покажите, что операторы $E_{ij} = a_i^* a_j, i, j = 1, ..., n$, удовлетворяют коммутационным соотношениям алгебры Ли $\mathrm{sl}(n, \mathbb{C})$.

6.4.4 Coherent States (??)

(об этом в главе про операторы также многое сказано)

Теория по Киселеву

Соотношение неопределенностей для двух наблюдаемых $\hat{A}$ и $\hat{B}$ минимизируется, если в гильбертовом пространстве квантовых состояний существует такое состояние $|\Psi\rangle$, что верно (см. (1.24)-(1.25))

$$(\hat{A} - \bar{A})|\Psi\rangle = \mathrm{i}\gamma(\hat{B} - \bar{B})|\Psi\rangle, \quad \gamma \in \mathbb{R}$$

где

$$\gamma = -2\mathrm{i}\frac{(\Delta A)^2}{\langle[\hat{A}, \hat{B}]\rangle} \Rightarrow |\gamma| = \frac{\Delta A}{\Delta B}$$

Для операторов $\hat{\mathcal{Q}}$ и $\hat{\mathcal{P}}$ согласно уравнению (1.24), где $\hat{A} \mapsto \hat{\mathcal{Q}}$ и $\hat{B} \mapsto \hat{\mathcal{P}}$, введем состояние $|\alpha\rangle$ в координатном представлении $\langle\mathcal{Q}|\alpha\rangle \equiv \psi_\alpha(\mathcal{Q})$, которое минимизирует соотношение неопределенностей со средними значениями $\langle\mathcal{Q}\rangle \equiv \langle\alpha|\mathcal{Q}|\alpha\rangle \equiv \mathcal{Q}_0$ и $\langle\mathcal{P}\rangle \equiv \langle\alpha|\mathcal{P}|\alpha\rangle \equiv \mathcal{P}_0$, и, следовательно,

$$(\mathcal{Q} - \mathcal{Q}_0)\,\psi_\alpha(\mathcal{Q}) = \mathrm{i}\gamma\left(-\mathrm{i}\frac{\partial}{\partial\mathcal{Q}} - \mathcal{P}_0\right)\psi_\alpha(\mathcal{Q}) \Leftrightarrow$$

$$\Leftrightarrow \left(\mathcal{Q} - \gamma\frac{\partial}{\partial\mathcal{Q}}\right)\psi_\alpha(\mathcal{Q}) = (\mathcal{Q}_0 - \mathrm{i}\gamma\mathcal{P}_0)\,\psi_\alpha(\mathcal{Q})$$

Это обыкновенное дифференциальное уравнение легко решается в общем виде, так как

$$\frac{\mathrm{d}\psi_\alpha}{\psi_\alpha} = \mathrm{d}\mathcal{Q}\frac{1}{\gamma}\,(\mathcal{Q} - \mathcal{Q}_0 + \mathrm{i}\gamma\mathcal{P}_0)$$

откуда

$$\psi_\alpha(\mathcal{Q}) = \psi_0 \mathrm{e}^{\frac{(\mathcal{Q}-\mathcal{Q}_0)^2}{2\gamma} + \mathrm{i}\mathcal{P}_0\mathcal{Q}},$$

и с учетом

$$\gamma = -2\mathrm{i}\frac{(\Delta\mathcal{Q})^2}{\langle[\hat{\mathcal{Q}}, \hat{\mathcal{P}}]\rangle} = -2(\Delta\mathcal{Q})^2$$

находим

$$\psi_\alpha(\mathcal{Q}) = \psi_0 \mathrm{e}^{-\frac{(\mathcal{Q}-\mathcal{Q}_0)^2}{4(\Delta\mathcal{Q})^2} + \mathrm{i}\mathcal{P}_0\mathcal{Q}}$$

Решение уравнения (6.29) является нормируемым и, следовательно, принадлежит гильбертову пространству только при $\gamma < 0$, и в этом случае говорят, что это решение - сжатое состояние (squeezed state) [1] для координаты, если $|\gamma| < 1$, или для импульса, если $|\gamma| > 1$. Особый случай при $\gamma = -1$ мы рассмотрим более подробно.

Итак, в общем случае соотношение неопределенностей координата-импульс минимизируется на волновых функциях гауссова типа с учетом наличия ненулевого среднего импульса, что приводит к стандартному множителю в виде волны де Бройля с фазой, зависящей от координаты и среднего значения импульса.

Для произвольной системы мы можем изготовить состояние гауссова типа, которое минимизирует соотношение неопределенностей координата-импульс в начальный момент времени. Но это не значит, что составленный таким образом волновой пакет сохранит это свойство минимизации в ходе эволюции: волновой пакет может расплыться, причем зависимость произведения дисперсий от времени определяется как гамильтонианом физической системы, так и параметрами начального состояния. Особый интерес представляют системы, для которых можно в явном виде построить динамически устойчивые волновые функции, минимизирующие соотношение неопределенностей координата-импульс во все моменты времени!

Итак, расплывание волнового пакета, минимизирующего соотношение неопределенностей координата-импульс, зависит, во-первых, от величины параметра γ, который входит в уравнение (6.29) и связан с параметром сжатия [1]

$$|\zeta| \stackrel{\text{def}}{=} -\frac{1}{2}\ln(-\gamma),$$

а во-вторых, от гамильтониана системы, задающего эволюцию волнового пакета.

Квантовые состояния, представляющие из себя нерасплывающиеся со временем гауссовы волновые пакеты, в максимальной степени соответствуют движению исходной классической системы. Именно такие квантовые состояния могут быть построены для физической системы с гамильтонианом гармонического осциллятора и называются когерентными: значение произведения дисперсий координаты и импульса минимально и не изменяется в ходе эволюции. Этого условия, в принципе, достаточно, чтобы, рассматривая эволюцию во времени дисперсии координаты и дисперсии импульса, точно построить когерентное состояние, но мы подойдем к этому вопросу менее формально и найдем основное уравнение когерентного состояния из описания состояний осциллятора.

Задача 3.1. Гармонический осциллятор в начальный момент времени находится в состоянии $|\alpha(\gamma)\rangle$, минимизирующем соотношение неопределенности координатаимпульс в осцилляторных единицах:

$$(\hat{\mathcal{Q}} - \mathrm{i}\gamma\hat{\mathcal{P}})|\alpha(\gamma)\rangle = (\langle\mathcal{Q}\rangle - \mathrm{i}\gamma\langle\mathcal{P}\rangle)|\alpha(\gamma)\rangle, \quad \gamma < 0.$$

Найдите значение параметра γ, при котором исходный волновой пакет не расплывается, т.е. флуктуации координаты и импульса остаются постоянными. Hits: - Используя исходное уравнение для состояния и коммутационные соотношения, запишите уравнение для бра-вектора состояния $\langle\alpha(\gamma)|$. Вычислите средние значения операторов $(\hat{\mathcal{Q}}-\mathrm{i}\gamma\hat{\mathcal{P}})(\hat{\mathcal{Q}}-\mathrm{i}\gamma\hat{\mathcal{P}})$ и $(\hat{\mathcal{Q}}+\mathrm{i}\gamma\hat{\mathcal{P}})(\hat{\mathcal{Q}}-\mathrm{i}\gamma\hat{\mathcal{P}})$ и получите дисперсии координаты и импульса, $(\Delta\mathcal{Q})^2$ и $(\Delta\mathcal{P})^2$ в начальный момент времени в теминах параметра γ. - Используя уравнение Гейзенберга и теорему Эренфеста для осциллятора, вычислите производные по времени

$$\frac{\mathrm{d}}{\mathrm{d}t}(\Delta\mathcal{Q})^2, \quad \frac{\mathrm{d}}{\mathrm{d}t}(\Delta\mathcal{P})^2$$

в начальный момент времени. - Вычислите вторые производные по времени

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}(\Delta\mathcal{Q})^2, \quad \frac{\mathrm{d}^2}{\mathrm{d}t^2}(\Delta\mathcal{P})^2$$

в начальный момент времени. - Найдите значение γ, при котором вторые производные тождественно обращаются в нуль в начальный момент времени. - Покажите, что все высшие производные в начальный момент времени также равны нулю.

Заметим, что стационарное вакуумное состояние осциллятора $\psi_0(\mathcal{Q})$ с энергией $E_0 = \hbar\omega/2$ является гауссовым волновым пакетом с

$$(\Delta\mathcal{Q})^2 = \frac{1}{2} \Rightarrow \gamma = -1.$$

В силу стационарности этого состояния, эволюция сводится к элементарной зависимости от времени в виде множителя $\mathrm{e}^{-\mathrm{i}E_0 t/\hbar}$,

$$\psi_0(t, \mathcal{Q}) = \mathrm{e}^{-\mathrm{i}\omega t/2}\psi_0(\mathcal{Q}),$$

а значит, волновой пакет остается гауссовым, и эта гауссова форма зависимости от координаты $\mathcal{Q}$ не изменяется со временем, и стало быть, свойство минимизации является динамически устойчивым. Это позволяет нам определить, по отношению к какому значению параметра γ состояния осциллятора, минимизирующие соотношение неопределенностей координата-импульс, являются сжатыми. Мы полагаем $\gamma_0 = -1$, как у вакуума - состояния с нулевым числом квантов энергии. При $\gamma = -1$ уравнение (6.30) перепишется в виде

$$\left(\mathcal{Q} + \frac{\partial}{\partial\mathcal{Q}}\right)\psi_\alpha(\mathcal{Q}) = (\mathcal{Q}_0 + \mathrm{i}\mathcal{P}_0)\,\psi_\alpha(\mathcal{Q})$$

Учитывая явное выражение для оператора $\hat{a}$ в представлении наблюдаемой координаты $\{\mathcal{Q}\}$, находим

$$\hat{a}\psi_\alpha(\mathcal{Q}) = \alpha\psi_\alpha(\mathcal{Q}), \quad \alpha = \frac{1}{\sqrt{2}}\left(\mathcal{Q}_0 + \mathrm{i}\mathcal{P}_0\right).$$

В обозначениях Дирака уравнение (6.32) может быть представлено как уравнение на собственные значения оператора уничтожения квантов

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$$

причем комплексное собственное значение имеет вполне определенный физический смысл: с точностью до фактора $\sqrt{2}$ вещественная часть собственного значения есть среднее значение координаты осциллятора, а мнимая часть среднее значение импульса.

Кроме того, вычисляя квадрат вектора состояния (6.34), находим, с одной стороны,

$$(\hat{a}|\alpha\rangle)^\dagger\hat{a}|\alpha\rangle = \left\langle\alpha\left|\hat{a}^\dagger\hat{a}\right|\alpha\right\rangle = \langle\alpha|\hat{N}|\alpha\rangle,$$

а с другой-

$$(\hat{a}|\alpha\rangle)^\dagger\hat{a}|\alpha\rangle = |\alpha|^2\langle\alpha|\alpha\rangle = |\alpha|^2,$$

где мы учли нормировку состояния на единицу. Значит,

$$\langle N\rangle = |\alpha|^2,$$

т. е. среднее число квантов в таком состоянии определяется квадратом модуля собственного значения оператора уничтожения.

Покажем теперь, что сжатые состояния, заданные уравнением (6.34), с коэффициентом сжатия $|\zeta| = 0$ или $\gamma = -1$, являются когерентными, т. е. они остаются сжатыми с тем же коэффициентом сжатия в ходе эволюции с гамильтонианом гармонического осциллятора.

Разложение по базису

Коммутатор оператора уничтожения с гамильтонианом

$$[\hat{H}, \hat{a}] = \hbar\omega \left[\hat{a}^\dagger \hat{a}, \hat{a}\right] = -\hbar\omega \left[\hat{a}, \hat{a}^\dagger\right] \hat{a} = -\hbar\omega\hat{a}$$

не обращается в нуль (за исключением среднего значения для вакуумного состояния). Поэтому энергия в состоянии $|\alpha\rangle$ флуктуирует вблизи своего среднего значения, определенного согласно (6.35) : $\langle E\rangle = \hbar\omega(\langle N\rangle + 1/2)$. Разложим это состояние по базису стационарных фоковских состояний

$$|\alpha\rangle = \sum_n C_n(\alpha)|n\rangle$$

У множим это разложение на бра-вектор $\langle n|$ и учтём уравнения на собственные значения

$$C_n(\alpha) = \langle n|\alpha\rangle = \frac{1}{\alpha}\langle n|\hat{a}\alpha\rangle = \frac{1}{\alpha}\left\langle \hat{a}^\dagger n|\alpha\right\rangle,$$

где мы воспользовались также определением операции эрмитова сопряжения оператора. По построению

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

так что получаем рекуррентное соотношение

$$\alpha C_n(\alpha) = \sqrt{n+1}C_{n+1}(\alpha)$$

которое можно разрешить в явном виде:

$$C_n(\alpha) = \frac{\alpha^n}{\sqrt{n!}}C_0(\alpha)$$

Разложение принимает вид

$$|\alpha\rangle = C_0(\alpha)\sum_n \frac{\alpha^n}{\sqrt{n!}}|n\rangle = C_0(\alpha)\sum_n \frac{\left(\alpha\hat{a}^\dagger\right)^n}{n!}|0\rangle = C_0(\alpha)\mathrm{e}^{\alpha\hat{a}^\dagger}|0\rangle$$

где мы использовали соотношение

$$|n\rangle = \frac{\left(\hat{a}^\dagger\right)^n}{\sqrt{n!}}|0\rangle$$

Коэффициент $C_0(\alpha)$ можно определить из условия единичной нормировки состояния (6.36)

$$\langle\alpha|\alpha\rangle = |C_0(\alpha)|^2\sum_n \frac{(\alpha^*\alpha)^n}{n!} = 1,$$

где мы учли ортонормированность стационарных состояний. Отсюда

$$|C_0(\alpha)|^2\,\mathrm{e}^{|\alpha|^2} = 1 \Rightarrow C_0(\alpha) = \mathrm{e}^{-\frac{|\alpha|^2}{2}},$$

когерентные состояния - фундаментальное понятие

(?? почему???)

Applications of coherent states

(there are a lot of them, see note on q opt for now about them, I'll write later)

6.4.5 Oscillator in the Holomorphic Representation

Зачем нужно голоморфное представление? (?????)

(this is a important question for understanding this topic, I'll think about it later)

Осциллятор в голоморфном представлении по Киселеву (??)

Наряду с задачей нахождения амплитуды вероятности перехода из точки в точку, можно поставить другую задачу: в зависимости от времени вычислить амплитуду вероятности перехода между фоковскими состояниями или, в самом общем виде, из одного когерентного состояния в другое. Тогда вместо координатного и импульсного представлений нужно использовать базис когерентных состояний $|\alpha\rangle$ с комплексным параметром $\alpha \in \mathbb{C}$, или, как говорят, рассмотреть задачу в пространстве Баргмана-Фока:

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle, \quad \int |\alpha\rangle \frac{\mathrm{d}\bar{\alpha}\mathrm{d}\alpha}{2\pi\mathrm{i}}\langle\alpha| = \mathbb{1}, \quad \langle\alpha'|\alpha\rangle = \exp\left\{-\frac{\bar{\alpha}'\alpha'}{2} - \frac{\bar{\alpha}\alpha}{2} + \bar{\alpha}'\alpha\right\}.$$

Для построения интеграла по траекториям в голоморфном представлении, как теперь понятно из проведенного выше общего анализа, необходимо рассмотреть оператор эволюции на k-м шаге разбиения интервала времени от t' до t''

$$\hat{U}\left(t_k + \mathrm{d}t, t_k\right) = \int |\alpha_{k+1}\rangle \frac{\mathrm{d}\bar{\alpha}_{k+1}\ \mathrm{d}\alpha_{k+1}}{2\pi\mathrm{i}} \left\langle \alpha_{k+1} \left| \hat{U}\left(t_k + \mathrm{d}t, t_k\right) \right| \alpha_k \right\rangle \frac{\mathrm{d}\bar{\alpha}_k\ \mathrm{d}\alpha_k}{2\pi\mathrm{i}} \langle\alpha_k| .$$

С точностью до членов второго порядка малости по шагу эволюции $\mathrm{d}t \to 0$ матричный элемент оператора эволюции

$$\left\langle \alpha_{k+1} \left| \hat{U}\left(t_k + \mathrm{d}t, t_k\right) \right| \alpha_k \right\rangle = \left\langle \alpha_{k+1} \left| \mathbb{1} - \frac{\mathrm{i}}{\hbar}\hat{H}\left(\hat{a}^\dagger, \hat{a}, t_k\right)\mathrm{d}t \right| \alpha_k \right\rangle$$

где необходимо вычислить матричный элемент гамильтониана, используя выражение для гамиьлтониана через операторы рождения и уничтожения, действие которых на квантовые состояния определены соответственно для бра- и кет-векторов, и мы найдем,

$$\left\langle \alpha_{k+1} \left| \hat{H}\left(\hat{a}^\dagger, \hat{a}, t_k\right) \right| \alpha_k \right\rangle = \mathcal{H}\left(\bar{\alpha}_{k+1}, \alpha_k, t_k\right) \langle\alpha_{k+1}|\alpha_k\rangle$$

если гамильтониан, как говорят, нормально упорядочен: все операторь рождения стоят слева от операторов уничтожения. В этом случае действие операторов уничтожения на кет-вектор когерентного состояния дает собственные значения

$$\hat{a}\,|\alpha_k\rangle = \alpha_k\,|\alpha_k\rangle$$

и аналогично для бра-векторов

$$\langle\alpha_{k+1}|\,\hat{a}^\dagger = \langle\alpha_{k+1}|\,\bar{\alpha}_{k+1}$$

Например, для свободного осциллятора

$$\hat{H}_0 = \hbar\omega_0\hat{a}^\dagger\hat{a} + \frac{1}{2}\hbar\omega_0$$

и

$$\left\langle \alpha_{k+1} \left| \hat{H}_0 \right| \alpha_k \right\rangle = \left\{\hbar\omega_0\bar{\alpha}_{k+1}\alpha_k + \frac{1}{2}\hbar\omega_0\right\}\langle\alpha_{k+1}|\alpha_k\rangle$$

Тогда

$$\left\langle \alpha_{k+1} \left| \hat{U}\left(t_k + \mathrm{d}t, t_k\right) \right| \alpha_k \right\rangle = \left\langle \alpha_{k+1} \left| \mathbb{1} - \frac{\mathrm{i}}{\hbar} \hat{H}\left(\hat{a}^\dagger, \hat{a}, t_k\right) \mathrm{d}t \right| \alpha_k \right\rangle =$$
$$= \langle \alpha_{k+1} | \alpha_k \rangle \left\{ 1 - \frac{\mathrm{i}}{\hbar} \mathcal{H}\left(\bar{\alpha}_{k+1}, \alpha_k, t_k\right) \mathrm{d}t \right\} =$$
$$= \langle \alpha_{k+1} | \alpha_k \rangle \exp\left\{ -\frac{\mathrm{i}}{\hbar} \mathcal{H}\left(\bar{\alpha}_{k+1}, \alpha_k, t_k\right) \mathrm{d}t \right\}$$

Матричный элемент $\langle \alpha_{k+1} | \alpha_k \rangle$ был определен при построении когерентных состояний осциллятора:

$$\langle \alpha_{k+1} | \alpha_k \rangle = \exp\left\{ -\frac{\bar{\alpha}_{k+1}\alpha_{k+1}}{2} - \frac{\bar{\alpha}_k \alpha_k}{2} + \bar{\alpha}_{k+1}\alpha_k \right\}$$

который можно представить в виде

$$\langle \alpha_{k+1} | \alpha_k \rangle = \exp\left\{ \frac{1}{2}\left(\bar{\alpha}_{k+1} - \bar{\alpha}_k\right)\alpha_k - \frac{1}{2}\bar{\alpha}_{k+1}\left(\alpha_{k+1} - \alpha_k\right) \right\}.$$

Поскольку множества точек $\{\bar{\alpha}_k, \alpha_k\}$ по построению соответствуют траекториям $\{\bar{\alpha}(t), \alpha(t)\}$, естественно ввести скорости изменения параметров траекторий

$$\left(\bar{\alpha}_{k+1} - \bar{\alpha}_k\right) = \dot{\bar{\alpha}}\left(t_k\right) \mathrm{d}t, \quad \left(\alpha_{k+1} - \alpha_k\right) = \dot{\alpha}\left(t_k\right) \mathrm{d}t$$

Значит,

$$\langle \alpha_{k+1} | \alpha_k \rangle = \exp\left\{ \frac{1}{2}\left[\dot{\bar{\alpha}}\left(t_k\right)\alpha\left(t_k\right) - \bar{\alpha}\left(t_k\right)\dot{\alpha}\left(t_k\right)\right] \mathrm{d}t \right\}$$

Таким образом, бесконечно малый шаг эволюции

$$\hat{U}\left(t_k + \mathrm{d}t, t_k\right) = \int |\alpha_{k+1}\rangle \frac{\mathrm{d}\bar{\alpha}_{k+1}\, \mathrm{d}\alpha_{k+1}}{2\pi\mathrm{i}} \left\langle \alpha_{k+1} \left| \hat{U}\left(t_k + \mathrm{d}t, t_k\right) \right| \alpha_k \right\rangle \frac{\mathrm{d}\bar{\alpha}_k\, \mathrm{d}\alpha_k}{2\pi\mathrm{i}} \langle \alpha_k |$$

представим в виде

$$\hat{U}\left(t_k + \mathrm{d}t, t_k\right) = \int |\alpha_{k+1}\rangle \frac{\mathrm{d}\bar{\alpha}_{k+1}\, \mathrm{d}\alpha_{k+1}}{2\pi\mathrm{i}} \frac{\mathrm{d}\bar{\alpha}_k\, \mathrm{d}\alpha_k}{2\pi\mathrm{i}} \langle \alpha_k | \times$$
$$\times \exp\left\{ \frac{\mathrm{i}}{\hbar} \mathrm{d}t \left[-\frac{\mathrm{i}\hbar}{2}\left[\dot{\bar{\alpha}}\left(t_k\right)\alpha\left(t_k\right) - \bar{\alpha}\left(t_k\right)\dot{\alpha}\left(t_k\right)\right] - \mathcal{H}\left(\bar{\alpha}\left(t_k\right), \alpha\left(t_k\right), t_k\right) \right] \right\}$$

а на конечном интервале времени

$$\hat{U}\left(t'', t'\right) = \lim_{N\to\infty} \int \frac{\mathrm{d}\bar{\alpha}_N\, \mathrm{d}\alpha_N}{2\pi\mathrm{i}} \frac{\mathrm{d}\bar{\alpha}_1\, \mathrm{d}\alpha_1}{2\pi\mathrm{i}} |\alpha_N\rangle \langle \alpha_1 | \int \prod_{k=2}^{N-1} \frac{\mathrm{d}\bar{\alpha}_k\, \mathrm{d}\alpha_k}{2\pi\mathrm{i}} \times$$
$$\times \exp\left\{ \frac{\mathrm{i}}{\hbar} \int_{t'}^{t''} \mathrm{d}t \left[-\frac{\mathrm{i}\hbar}{2}[\dot{\bar{\alpha}}(t)\alpha(t) - \bar{\alpha}(t)\dot{\alpha}(t)] - \mathcal{H}(\bar{\alpha}(t), \alpha(t), t) \right] \right\}$$

где интегрирование по времени дает действие на траектории в классической механике. В самом деле, вклад

$$\int p(t)\dot{q}(t)\mathrm{d}t$$

можно после интегрирования по частям представить как

$$\frac{1}{2}\int [p(t)\dot{q}(t) - q(t)\dot{p}(t)]\mathrm{d}t$$

Тогда стандартная замена переменных

$$q(t) = \sqrt{\frac{\hbar}{m\omega_0}}\frac{1}{\sqrt{2}}[\bar{\alpha}(t) + \alpha(t)], \quad p(t) = \sqrt{\hbar m\omega_0}\frac{\mathrm{i}}{\sqrt{2}}[\bar{\alpha}(t) - \alpha(t)]$$

после приведения подобных членов дает

$$\frac{1}{2}\int [p(t)\dot{q}(t) - q(t)\dot{p}(t)]\mathrm{d}t = -\int \mathrm{d}t\frac{\mathrm{i}\hbar}{2}[\dot{\bar{\alpha}}(t)\alpha(t) - \bar{\alpha}(t)\dot{\alpha}(t)].$$

Из 13.53 в пределе $N \to \infty$ получаем интеграл по траекториям в представлении когерентных состояний

$$\hat{U}\left(t'', t'\right) = \int \frac{\mathrm{d}\bar{\alpha}\left(t''\right)\mathrm{d}\alpha\left(t''\right)}{2\pi\mathrm{i}}\frac{\mathrm{d}\bar{\alpha}\left(t'\right)\mathrm{d}\alpha\left(t'\right)}{2\pi\mathrm{i}}\left|\alpha\left(t''\right)\right\rangle\left\langle\alpha\left(t'\right)\right| \int \mathcal{D}\bar{\alpha}\mathcal{D}\alpha \cdot \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t'',t')},$$

где действие на траектории

$$S\left(t'', t'\right) = \int_{t'}^{t''} \mathrm{d}t\left[-\frac{\mathrm{i}\hbar}{2}[\dot{\bar{\alpha}}(t)\alpha(t) - \bar{\alpha}(t)\dot{\alpha}(t)] - \mathcal{H}(\bar{\alpha}(t), \alpha(t), t)\right].$$

Так же, как в координатно-импульсном представлении континуального интеграла интегрирование в фазовом пространстве по траектории импульса было независимым от интегрирования по траектории координаты (импульс не определяется скоростью!), в голоморфном представлении траектории $\bar{\alpha}(t)$ и $\alpha(t)$ не связаны комплексным сопряжением, а являются независимыми однопараметрическими кривыми в двух комплексных плоскостях z и $w : z$ для α и w для $\bar{\alpha}$.

Ядро оператора. Для определения голоморфного представления оператора $\hat{A}$ запишем:

$$\hat{A} = \int \left|\alpha_{\text{out}}\right\rangle \frac{\mathrm{d}\bar{\alpha}_{\text{out}}\,\mathrm{d}\alpha_{\text{out}}}{2\pi\mathrm{i}}\left\langle\alpha_{\text{out}}\left|\hat{A}\right|\alpha_{\text{in}}\right\rangle \frac{\mathrm{d}\bar{\alpha}_{\text{in}}\,\mathrm{d}\alpha_{\text{in}}}{2\pi\mathrm{i}}\left\langle\alpha_{\text{in}}\right|,$$

причем матричный элемент можно определить с помощью полного набора собственных состояний энергии для осциллятора

$$\left\langle\alpha_{\text{out}}\left|\hat{A}\right|\alpha_{\text{in}}\right\rangle = \sum_{n,m}\left\langle\alpha_{\text{out}}\left|n\right\rangle\right\langle n|\hat{A}|m\rangle\left\langle m|\alpha_{\text{in}}\right\rangle = \\ = \sum_{n,m}\frac{\bar{\alpha}_{\text{out}}^n}{\sqrt{n!}}A_{nm}\frac{\alpha_{\text{in}}^m}{\sqrt{m!}}\cdot\exp\left\{-\frac{\bar{\alpha}_{\text{out}}\,\alpha_{\text{out}}}{2} - \frac{\bar{\alpha}_{\text{in}}\alpha_{\text{in}}}{2}\right\},$$

где мы стандартно ввели матричные элементы оператора $A_{nm} = \langle n|\hat{A}|m\rangle$ и воспользовались голоморфным представлением для волновых функций собственных состояний энергии осциллятора. Поэтому голоморфное ядро оператора определяют в полной аналогии с волновыми функциями

$$\mathcal{A}\left(\bar{\alpha}_{\text{out}}, \alpha_{\text{in}}\right) = \left\langle\alpha_{\text{out}}\left|\hat{A}\right|\alpha_{\text{in}}\right\rangle \cdot \mathrm{e}^{\frac{\bar{\alpha}_{\text{Out}}\,\alpha_{\text{out}}}{2} + \frac{\bar{\alpha}_{\text{in}}\alpha_{\text{in}}}{2}} = \sum_{n,m}\frac{\bar{\alpha}_{\text{out}}^n}{\sqrt{n!}}A_{nm}\frac{\alpha_{\text{in}}^m}{\sqrt{m!}},$$

и оно действительно, как мы только что показали, является функцией только от $\bar{\alpha}_{\text{out и}}\,\alpha_{\text{in}}$ и не зависит от переменных, комплексно сопряженных к ним!

В частности, голоморфное ядро оператора эволюции имеет вид

$$\mathcal{U}\left(\bar{\alpha}_{\text{out}}\,,\alpha_{\text{in}}\right)=\int\mathcal{D}\bar{\alpha}\mathcal{D}\alpha\cdot\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t'',t')}\cdot\mathrm{e}^{\frac{\bar{\alpha}_{\text{out}}\,\alpha_{\text{out}}}{2}+\frac{\bar{\alpha}_{\text{in}}\alpha_{\text{in}}}{2}},$$

где граничные условия задаются равенствами

$$\bar{\alpha}_{\text{out}}\,=\bar{\alpha}\left(t''\right),\quad\alpha_{\text{in}}=\alpha\left(t'\right)$$

Для рассмотрения граничных условий при наличии источников мы будем полагать, что $t'\to-\infty$ и $t''\to+\infty$, а сами источники отличны от нуля только при конечных временах (или достаточно быстро стремятся к нулю на временной бесконечности). Тогда состояния осциллятора в бесконечном прошлом и бесконечном будущем представимы в базисе собственных векторов энергии свободного осциллятора, т. е. в базисе с заданным числом квантов в начальном и конечном состоянии эволюции. тот базис определяет асимптотическое пространство состояний, а матричнье элементы оператора эволюции

$$\mathcal{S}_{nm}=\left\langle n\left|\hat{U}\left(t'',t'\right)\right|m\right\rangle\Big|_{j=0},\quad t'\to-\infty,t''\to+\infty$$

называют элементами «S-матрицы». Напомним, что гипотеза существования асимптотических состояний является ключевой при формулировке квантовой теории взаимодействующих полей, и фактически она может быть обоснована только после нахождения точного решения динамических уравнений теории, что на практике редко представляется возможным для реальных физических ситуаций, предоставленных нам природой [имеются искусственные примеры точных решений, например, электродинамика частицы с половинным спином в одном пространственном измерении (модель Швингера)]. Математически строго этот вопрос рассматривается в рамках аксиоматического подхода 1. S-матрица не является уже, вообще говоря, диагональной, так как при наличии взаимодействия количество квантов разного сорта (если осцилляторов несколько) может изменяться (поглощаться и излучаться). Особый случай вакуум. Мыл будем считать, что вакуум стабияен. Это означает, что в ходе эволюции вакуум переходит в себя с вероятностью, равной единице, а значит, модуль амплитуды перехода равен единице:

$$\left|\left\langle 0\left|\hat{U}\left(t'',t'\right)\right|0\right\rangle\right|=1,\quad t'\to-\infty,t''\to+\infty$$

Другими словами, эволюция вакуума сводится к введению фазового множителя, который вообще зависит от источников как функционал, и этот фактор обычно полагают равным единице в отсутствие источников [2], Поэтому для

[1] См., например, Боголюбов Н. Н., Логунов А. А., Оксак А. И., Тодо р о в И. Т. Общие принципы квантовой теории поля. М.: Наука, 1987).

2 то означает, что мы производим сдвиг энергии вакуума: $E_0=\frac{1}{2}\hbar\omega_0\to E_{\text{vac}}=0$, - так что она принимается равной нулю. вакуума

$$|\text{ out }\rangle=\hat{U}|\text{ in }\rangle=\mathrm{e}^{\frac{\mathrm{i}}{\hbar}G[j]}|\text{ in }\Big\rangle,\quad|\text{ in }\Big\rangle=|0\rangle$$

т. е. состояния «in» и «out» совпадают с точностью до фазы, которую мы определим позже с помощью введения нового понятия - производящего функционала связных функций Грина $G[j]$. Значит,

$$\langle\text{out}|=\langle\text{in}\,|\hat{U}^{\dagger}$$

Поэтому Т-произведения операторов, которые выражаются через интеграл по траекториям, при $t_1>t_2$

$$\left\langle \text{ out } \left| \hat{U}\hat{F}_H\left(t_1\right)\hat{G}_H\left(t_2\right) \right| \text{ in } \right\rangle = \left\langle \text{ in } \left| \hat{F}_H\left(t_1\right)\hat{G}_H\left(t_2\right) \right| \text{ in } \right\rangle$$

Элементы $\mathcal{S}$-матрицы можно выразить через производные голоморфного ядра оператора эволюции при нулевых источниках, поскольку

$$\mathcal{U}\left(\bar{\alpha}_{\text{out}}\,,\alpha_{\text{in}}\right) = \sum_{n,m} \frac{\bar{\alpha}_{\text{out}}^n}{\sqrt{n!}} U_{nm} \frac{\alpha_{\text{in}}^m}{\sqrt{m!}}$$

так что

$$\begin{aligned}\mathcal{S}_{nm} &= \frac{1}{\sqrt{n!m!}}\,\frac{\partial^{n+m}}{\partial\bar{\alpha}_{\text{out}}^n\,\partial\alpha_{\text{in}}^m}\mathcal{U}\left(\bar{\alpha}_{\text{out}}\,,\alpha_{\text{in}}\right)\Big|_{\bar{\alpha}_{\text{out}}=\alpha_{\text{in}}=0} = \\ &= \frac{1}{\sqrt{n!m!}}\frac{\partial^{n+m}}{\partial\bar{\alpha}_{\text{out}}^n\,\partial\alpha_{\text{in}}^m}\int \mathcal{D}\bar{\alpha}\mathcal{D}\alpha\cdot \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t'',t')}\cdot \mathrm{e}^{\frac{\bar{\alpha}_{\text{Out}}\,\alpha_{\text{out}}}{2}+\frac{\bar{\alpha}_{\text{in}}\alpha_{\text{in}}}{2}}\Big|_{\bar{\alpha}_{\text{out}}=\alpha_{\text{in}}=0}.\end{aligned}$$

При расчете переходов из вакуума в вакуум дополнительные множители исчезают, а $\alpha_{\text{in}}\,,\bar{\alpha}_{\text{out}}\,\to 0$

$$\langle 0|\hat{U}|0\rangle = \mathcal{U}(0,0)$$

и при наличии источников так же.

При переходе «вакуум-вакуум» матричный элемент оператора эволюции выражается через интеграл по траекториям

$$\left\langle 0\left|\hat{U}\left(t'',t'\right)\right|0\right\rangle = \int \mathcal{D}\bar{\alpha}\mathcal{D}\alpha\cdot \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t'',t')},\quad t'\to-\infty, t''\to+\infty.$$

При этом начальные данные отвечают $\alpha\left(t'\right) = \alpha_{\text{in}} \equiv 0$, а конечные данные $\bar{\alpha}\left(t''\right) = \bar{\alpha}_{\text{out}} \equiv 0$. Важно подчеркнуть, что α_{in} является собственным значением для оператора уничтожения квантов в начальном состоянии, и при бесконечно малом шаге эволюции от исходного состояния в выражении для матричного элемента оператора эволюции не возникает сопряженное собственное значение $\bar{\alpha}_{\text{in}}$, а в это выражение входит независимая величина $\bar{\alpha}\left(t'+\mathrm{d}t\right)$. И аналогично $\bar{\alpha}_{\text{out}}$ - это собственное значение для оператора рождения, который действует на бра-вектор конечного состояния, и в выражении для матричного элемента оператора эволюции не возникает собственное значение α_{out} . Другими словами, у нас есть две комплексные плоскости с траекториями $\alpha(t)$ и $\bar{\alpha}(t)$, и для этих траекторий зафиксированы начальная точка $\alpha\left(t'\right) = \alpha_{\text{in}}$ на плоскости $\alpha(t)$ и конечная точка $\bar{\alpha}\left(t''\right) = \bar{\alpha}_{\text{out}}$ на плоскости $\bar{\alpha}(t)$.

Модъ. Поскольку в голоморфном представлении состояния с заданным числом квантов являются собственными векторами оператора рождения с собственными значениями $\bar{\alpha}$:

$$\hat{a}^\dagger\psi_n(\bar{\alpha}) = \bar{\alpha}\psi_n(\bar{\alpha})$$

зависимость от времени параметров $\bar{\alpha}$ повторяет зависимость от времени оператора рождения

$$\hat{a}^\dagger(t) = \mathrm{e}^{\mathrm{i}\omega_0 t}\hat{a}^\dagger \Rightarrow \bar{\alpha}(t) = \mathrm{e}^{\mathrm{i}\omega_0 t}\bar{\alpha},\quad \alpha(t) = \mathrm{e}^{-\mathrm{i}\omega_0 t}\alpha$$

так что с учетом граничных условий $\bar{\alpha}\left(t''\right) = \bar{\alpha}_{\text{out}}\,,\alpha\left(t'\right) = \alpha_{\text{in}}$ находим

- при $t\to t''$, т. е. в асимптотическом будущем 1,

$$q(t) = x_0[\bar{\alpha}(t) + \alpha(t)] \to x_0 \left[\mathrm{e}^{-\mathrm{i}\omega_0 t}\alpha + \mathrm{e}^{\mathrm{i}\omega_0(t-t'')}\bar{\alpha}_{\mathrm{out}} \right]$$

с учетом $\bar{\alpha}_{\mathrm{out}} \to 0$ означает, что

$$q(t) \to x_0 \mathrm{e}^{-\mathrm{i}\omega_0 t}\alpha$$

т. е. в асимптотическом будущем распространяются только положительночастотные моды [2]

- при $t \to t'$, т. е. в асимптотическом прошлом [3]

$$q(t) = x_0[\bar{\alpha}(t) + \alpha(t)] \to x_0 \left[\mathrm{e}^{-\mathrm{i}\omega_0(t-t')}\alpha_{\mathrm{in}} + \mathrm{e}^{\mathrm{i}\omega_0 t}\bar{\alpha} \right]$$

с учетом $\alpha_{\mathrm{in}} \to 0$ означает, что

$$q(t) \to x_0 \mathrm{e}^{\mathrm{i}\omega_0 t}\bar{\alpha}$$

т. е. в асимптотическом прошлом распространяются только отрицательночастотные моды.

ти граничные условия позволят однозначно определить двухточечную функцию Грина для осциллятора при переходе «вакуум-вакуум», когда асимптотическое прошлое и будущее стремятся в бесконечность.

[1] Для краткости обозначим $x_0 = \sqrt{\hbar/\left(2m\omega_0\right)}\Big)$, так что само выражение в будущем отвечает матричному элементу оператора координаты по бра-состоянию $\langle \bar{\alpha}_{\mathrm{out}} \,|$ и по кетсостоянию на промежуточной стадии эволюции $|\alpha\rangle$.

[2] Наименование моды проистекает из вида зависимости волновой функции стационарного состояния от времени, которая задается зависящим от времени множителем $\exp(-\mathrm{i}Et/\hbar) = \exp(-\mathrm{i}\omega t)$, где энергия стационарного состояния $E = \hbar\omega$, так что положительная энергия отвечает положительной частоте, а экспоненциальный множитель имеет в своем аргументе отрицательный знак перед мнимой единицей.

[3] Рассматриваем решение для осциллятора, пропорциональное матричному элементу координаты между бра-состоянием на промежуточной стадии эволюции $\langle\alpha|$ и начальным кет-состоянием $|\alpha_{\mathrm{in}}\rangle$. Лекция 14 (дополнительная)

Континуальный интеграл при наличии источника, уравнения Швингера-Дайсона, производящие функционалы амплитуды $Z[j]$ и функций Грина $G[j]$, решение для осциллятора, причинный пропагатор Фейнмана и обход полюсов, теорема Вика, спаривания, 4-точка для осциллятора, теория возмущений и многоточечные корреляторы, диаграммы Фейнмана для трехточечного коррелятора в модели «лямбда-фи-в-кубе» в ведущем приближении, внешние и внутренние линии, вершины, компонентя связности диаграммы, диаграммы для многоточечных функций и источников, связные функции Грина, квантовый аналог классической траектории, преобразование Лежандра и квантовое эффективное действие, усеченные вершинные функции и диаграммы Фейнмана для уравнения Швингера-Дайсона в модели «лямбда-фи-в-четвертой», одночастичная неприводимость диаграмм в методе Коулмена-Вайнберга, связь числа петель с числом вершин и внутренних линий на связной диаграмме, разложение связных функций Грина по петлям и по степеням $\hbar$, графическое представление редукционных формул, пример введения взаимодействия осцилляторов.

7. Голоморфное представление и виковские символы

Рассмотрим гильбертово пространство

$$\ell^2 = \left\{ c = \{c_n\}_{n=0}^{\infty} : \|c\|^2 = \sum_{n=0}^{\infty} |c_n|^2 < \infty \right\}$$

последовательностей с суммируемым квадратом. Выбором ортонормального базиса $\{\psi_n\}_{n=0}^{\infty}$ в $L^2(\mathbb{R}, dq)$, состоящего из собственных функций (2.40) оператора Шрёдингера гармонического осциллятора, устанавливается изоморфизм гильбертовых пространств $L^2(\mathbb{R}, dq) \simeq \ell^2$

$$L^2(\mathbb{R}, dq) \ni \psi = \sum_{n=0}^{\infty} c_n \psi_n \mapsto c = \{c_n\}_{n=0}^{\infty} \in \ell^2$$

где

$$c_n = (\psi, \psi_n) = \int_{-\infty}^{\infty} \psi(q)\psi_n(q)dq$$

поскольку функции ψ_n вещественнозначны. Используя (2.39), получаем

$$a^*\psi = \sum_{n=0}^{\infty} c_n a^* \psi_n = \sum_{n=0}^{\infty} \sqrt{n+1} c_n \psi_{n+1} = \sum_{n=1}^{\infty} \sqrt{n} c_{n-1} \psi_n, \quad \psi \in D\left(a^*\right)$$

и

$$a\psi = \sum_{n=0}^{\infty} c_n a \psi_n = \sum_{n=1}^{\infty} \sqrt{n} c_n \psi_{n-1} = \sum_{n=0}^{\infty} \sqrt{n+1} c_{n+1} \psi_n, \quad \psi \in D(a)$$

так что в пространстве ℓ^2 операторы рождения и уничтожения a^* и a представлены следующими полубесконечными матрицами:

$$a = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad a^* = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

В результате

$$N = a^* a = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 2 & 0 & \cdots \\ 0 & 0 & 0 & 3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

так что гамильтониан гармонического осциллятора представлен диагональной матрицей

$$H = \hbar\omega \left(N + \frac{1}{2} \right) = \operatorname{diag} \left\{ \frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \ldots \right\}$$

Это представление коммутационных соотношений Гейзенберга называется представлением чисел заполнения и обладает тем свойством, что в нем гамильтониан H гармонического осциллятора диагонален.

Другое представление, в котором H диагонален, строится так. Пусть $\mathscr{D}$ - пространство целых функций $f(z)$ со скалярным произведением

$$(f,g)=\frac{1}{\pi}\int\limits_{\mathbb{C}} f(z)\overline{g(z)}e^{-|z|^2}d^2z$$

где $d^2z=\frac{i}{2}dz\wedge d\bar{z}$ - мера Лебега на $\mathbb{C}\simeq\mathbb{R}^2$. Легко проверить, что $\mathscr{D}$ - гильбертово пространство с ортонормальным базисом

$$f_n(z)=\frac{z^n}{\sqrt{n!}},\quad n=0,1,2,...$$

Соответствие

$$\ell^2\ni c=\{c_n\}_{n=0}^{\infty}\mapsto f(z)=\sum_{n=0}^{\infty}c_nf_n(z)\in\mathscr{D}$$

изоморфизм гильбертовых пространств $\ell^2\simeq\mathscr{D}$. Реализация гильбертова пространства $\mathscr{H}$ в виде гильбертова пространства $\mathscr{D}$ целых функций называется голоморфным представлением. В голоморфном представлении

$$a^*=z,\quad a=\frac{d}{dz},\qquad \text{и}\qquad H=\hbar\omega\left(z\frac{d}{dz}+\frac{1}{2}\right)$$

и очень легко показать, что a^* - оператор, сопряженный к a. Отображением

$$\mathscr{H}\ni\psi=\sum_{n=0}^{\infty}c_n\psi_n\mapsto f(z)=\sum_{n=0}^{\infty}c_nf_n(z)\in\mathscr{D}$$

устанавливается изоморфизм между координатным и голоморфным представлениями. Из формулы для производящей функции многочленов Эрмита-Чебышева,

$$\sum_{n=0}^{\infty}H_n(q)\frac{z^n}{n!}=e^{2qz-z^2}$$

следует, что соответствующий унитарный оператор $U:\mathscr{H}\to\mathscr{D}$ - это интегральный оператор

$$U\psi(z)=\int\limits_{-\infty}^{\infty}U(z,q)\psi(q)dq$$

с ядром

$$U(z,q)=\sum_{n=0}^{\infty}\psi_n(q)f_n(z)=\sqrt[4]{\frac{m\omega}{\pi\hbar}}e^{\frac{m\omega}{2\hbar}q^2-\left(\sqrt{\frac{m\omega}{\hbar}}q-\frac{1}{\sqrt{2}}z\right)^2}$$

Другая полезная реализация - представление в гильбертовом пространстве $\overline{\mathscr{D}}$ антиголоморфных функций $f(\bar{z})$ на $\mathbb{C}$ со скалярным произведением

задаваемое формулами

$$(f,g)=\frac{1}{\pi}\int\limits_{\mathbb{C}} f(\bar{z})\overline{g(\bar{z})}e^{-|z|^2}d^2z$$

$$a^* = \bar{z}, \quad a = \frac{d}{d\bar{z}}$$

ЗАМЕЧАНИЕ. Голоморфное и антиголоморфное представления соответствуют разным выборам комплексной поляризации симплектического многообразия $\mathbb{R}^2$. По определению комплексная поляризация симплектического многообразия $(\mathscr{M}, \omega)$ - это интегрируемое распределение на $\mathscr{M}$ комплексных лагранжевых подпространств комплексифицированных векторных пространств $T_x\mathscr{M} \otimes_{\mathbb{R}} \mathbb{C}$. Как и понятие вещественной поляризации, понятие комплексной поляризации играет фундаментальную роль в геометрическом квантовании. В частности, голоморфное представление соответствует комплексному лагранжеву подпространству в $T_x\mathbb{R}^2 \otimes_{\mathbb{R}} \mathbb{C} \simeq \mathbb{C}^2$, заданному уравнением $z = 0$, где z и $\bar{z}$ - комплексные координаты на $\mathbb{C}^2$. (Заметим, что здесь $\bar{z}$ не является комплексно сопряженным к z !) Уравнение $\bar{z} = 0$ определяет комплексное лагранжево подпространство, соответствующее антиголоморфному представлению.

Антиголоморфное представление используется для введения так называемых виковских символов операторов. А именно: пусть A - оператор в $\overline{\mathscr{D}}$, являющийся многочленом с постоянными коэффициентами в операторах рождения и уничтожения a^* и a. Используя коммутационное соотношение (2.34), можно перетащить все операторы a^* налево от операторов a и представить A в виковской нормальной форме следующим образом:

$$A = \sum_{l,m} A_{lm} \left(a^*\right)^l a^m$$

По определению виковский символ $A(\bar{z}, z)$ оператора A - это

$$A(\bar{z}, z) = \sum_{l,m} A_{lm} \bar{z}^l z^m$$

Это ограничение многочлена $A(v, z)$ в переменных v и z на $v = \bar{z}$.

Чтобы определить виковские символы ограниченных операторов в $\overline{\mathscr{D}}$, рассмотрим семейство когерентных состояний (или векторов Пуассона) $\Phi_v \in \overline{\mathscr{D}}, v \in \mathbb{C}$, определенных формулой

$$\Phi_v(\bar{z}) = e^{v\bar{z}}, \quad z \in \mathbb{C}.$$

Они удовлетворяют свойствам

$$a\Phi_v = v\Phi_v \quad \text{и} \quad f(\bar{v}) = (f, \Phi_v), \quad f \in \overline{\mathscr{D}}, v \in \mathbb{C}.$$

Действительно, первое свойство тривиально, тогда как «воспроизводящее свойство» мгновенно следует из формулы

$$\Phi_v(\bar{z}) = \sum_{n=0}^{\infty} f_n(v) \bar{f}_n(\bar{z}),$$

где $\bar{f}_n(\bar{z}) = \overline{f_n(z)}, n = 0, 1, 2, ...,$ - ортонормальный базис $\overline{\mathscr{D}}$.

Имеем также

$$(f, g) = \frac{1}{\pi} \int_{\mathbb{C}} (f, \Phi_v) \overline{(g, \Phi_v)} e^{-|v|^2} d^2 v$$

Дальше, для оператора A в виковской нормальной форме (2.46) получаем, используя первое свойство в (2.48),

$$(A\Phi_z, \Phi_{\bar{v}}) = \sum_{l,m} A_{lm} \left((a^*)^l a^m \Phi_z, \Phi_{\bar{v}} \right) = \sum_{l,m} A_{lm} \left(a^m \Phi_z, a^l \Phi_{\bar{v}} \right) =$$
$$= A(v,z) \left(\Phi_z, \Phi_{\bar{v}} \right).$$

Поэтому

$$A(v,z) = \frac{(A\Phi_z, \Phi_{\bar{v}})}{(\Phi_z, \Phi_{\bar{v}})} = e^{-vz} \left(A\Phi_z, \Phi_{\bar{v}} \right),$$

так как из воспроизводящего свойства следует, что $(\Phi_z, \Phi_{\bar{v}}) = \Phi_z(v) = e^{vz}$.

Определение. Виковский символ $A(\bar{z}, z)$ ограниченного оператора A в гильбертовом пространстве $\bar{D}$ является ограничением на подпространство $v = \bar{z}$ целой функции $A(v,z)$ в переменных v и z, определенной формулой

$$A(v,z) = e^{-vz} \left(A\Phi_z, \Phi_{\bar{v}} \right).$$

В следующей теореме мы перечислим основные свойства виковских символов.

Th. 2.2.

Виковские символы ограниченных операторов в $\overline{\mathscr{D}}$ обладают следующими свойствами.

(i) Если $A(\bar{z}, z)$ - виковский символ оператора A, то для виковского символа оператора A^* имеем $A^*(\bar{z}, z) = \overline{A(\bar{z}, z)}u$

$$A^*(v,z) = \overline{A(\bar{z}, \bar{v})}$$

(ii) Для $f \in \overline{\mathscr{D}}$

$$(Af)(\bar{z}) = \frac{1}{\pi} \int\limits_{\mathbb{C}} A(\bar{z}, v) f(\bar{v}) e^{-v(\bar{v}-\bar{z})} d^2 v$$

(iii) Вещественно-аналитическая функция $A(\bar{z}, z)$ является виковским символом ограниченного оператора A в $\overline{\mathscr{D}}$, если и только если она есть ограничение на подпространство $v = \bar{z}$ целой функции $A(v,z)$ в переменных v и z со свойством, что для любого $f \in \mathscr{D}$ интеграл в части (ii) абсолютно сходится и определяет функцию в $\overline{\mathscr{D}}$.

(iv) Если $A_1(\bar{z}, z)$ и $A_2(\bar{z}, z)$ - виковские символы операторов A_1 и A_2, то виковский символ оператора $A = A_1 A_2$ задается формулой

$$A(\bar{z}, z) = \frac{1}{\pi} \int\limits_{\mathbb{C}} A_1(\bar{z}, v) A_2(\bar{v}, z) e^{-(v-z)(\bar{v}-\bar{z})} d^2 v$$

ДОКАЗАТЕЛЬСТВО.

Имеем

$$A^*(v,z) = e^{-vz} \left(A^* \Phi_z, \Phi_{\bar{v}} \right) = e^{-vz} \left(\Phi_z, A\Phi_{\bar{v}} \right) = e^{-vz} \overline{(A\Phi_{\bar{v}}, \Phi_z)} = \overline{A(\bar{z}, \bar{v})}$$

что доказывает (i). Для доказательства (ii) воспользуемся воспроизводящим свойством и получим

$$(Af)(\bar{z}) = (Af, \Phi_z) = (f, A^* \Phi_z) = \frac{1}{\pi} \int\limits_{\mathbb{C}} f(\bar{v}) \overline{\left(A^* \Phi_z \right)(\bar{v})} e^{-|v|^2} d^2 v$$

Еще раз используя воспроизводящее свойство, получаем

$$\left(A^*\Phi_z\right)(\bar{v}) = \left(A^*\Phi_z, \Phi_v\right) = A^*(\bar{v}, z)\left(\Phi_z, \Phi_v\right) = \overline{e^{v\bar{z}}A(\bar{z}, v)}$$

что доказывает (ii). Свойство (iii) следует из определения и принципа равномерной ограниченности, который нужен, чтобы показать, что оператор A в $\bar{D}$, определенный интегралом в (ii), ограничен. Рутинные подробности остаются читателю. Чтобы доказать (iv), используя (2.50) и (i), мы получаем

$$\begin{aligned} A(\bar{z}, z) &= e^{-|z|^2}\left(A_1A_2\Phi_z, \Phi_z\right) = e^{-|z|^2}\left(A_2\Phi_z, A_1^*\Phi_z\right) = \\ &= \frac{1}{\pi}\int\limits_{\mathbb{C}}\left(A_2\Phi_z, \Phi_v\right)\overline{\left(A_1^*\Phi_z, \Phi_v\right)}e^{-\left(|v|^2+|z|^2\right)}d^2v = \\ &= \frac{1}{\pi}\int\limits_{\mathbb{C}}A_1(\bar{z}, v)A_2(\bar{v}, z)e^{-(v-z)(\bar{v}-\bar{z})}d^2v. \end{aligned}$$

ЗАмЕчАниЕ. Свойства (i) и (iv) остаются верными для многочленов от a^* и a - операторов вида (2.46).

Матричный символ $\tilde{A}(\bar{z}, z)$ ограниченного оператора A в гильбертовом пространстве $\overline{\mathscr{D}}$ - это ограничение на подпространство $v = \bar{z}$ целой функции $A(v, z)$ в переменных v и z, определенной следующим абсолютно сходящимся рядом:

$$\tilde{A}(v, z) = \sum_{m,n=0}^{\infty}\left(A\bar{f}_m, \bar{f}_n\right)f_n(v)f_m(z).$$

Матричный и виковский символы связаны следующим образом.

Лемма 2.4.

Для ограниченного оператора A в гильбертовом пространстве $\overline{\mathscr{D}}$

$$\tilde{A}(v, z) = e^{vz}A(v, z)$$

ДОКАЗАТЕЛЬСтвО.

Используя (2.49), получаем

$$\begin{aligned} \tilde{A}(v, z) &= \frac{1}{\pi}\sum_{m,n=0}^{\infty}f_n(v)f_m(z)\int\limits_{\mathbb{C}}\left(A\bar{f}_m\right)(\bar{u})f_n(u)e^{-|u|^2}d^2u = \\ &= \frac{1}{\pi}\int\limits_{\mathbb{C}}\left(A\Phi_z\right)(\bar{u})\overline{\Phi_{\bar{v}}(\bar{u})}e^{-|u|^2}d^2u = \left(A\Phi_z, \Phi_{\bar{v}}\right) = e^{vz}A(v, z). \end{aligned}$$

Перестановка суммирования и интегрирования корректна в виду абсолютной сходимости.

Следствие 2.3.

Если $\tilde{A}_1(\bar{z}, z)$ и $\tilde{A}_2(\bar{z}, z)$ - матричные символы операторов A_1 и A_2, то матричный символ оператора $A = A_1A_2$ дается формулой

$$\tilde{A}(\bar{z}, z) = \frac{1}{\pi}\int\limits_{\mathbb{C}}\tilde{A}_1(\bar{z}, v)\tilde{A}_2(\bar{v}, z)e^{-|v|^2}d^2v$$

ДОКАЗАТЕЛЬСТВО.

Доказательство мгновенно следует из части (iv) теоремы 2.2 и леммы 2.4.

Эти построения, очевидно, обобщаются на случай n степеней свободы. Гильбертово пространство $\mathscr{D}_n$, определяющее голоморфное представление, это пространство целых функций $f(\boldsymbol{z})$ от n комплексных переменных $\boldsymbol{z} = (z_1, ..., z_n)$ со скалярным произведением

$$(f, g) = \frac{1}{\pi^n} \int\limits_{\mathbb{C}^n} f(\boldsymbol{z})\overline{g(\boldsymbol{z})} e^{-|\boldsymbol{z}|^2} d^{2n}\boldsymbol{z} < \infty$$

где $|\boldsymbol{z}|^2 = z_1^2 + \cdots + z_n^2$ и $d^{2n}\boldsymbol{z} = d^2 z_1 \cdots d^2 z_n$ - мера Лебега на $\mathbb{C}^n \simeq \mathbb{R}^{2n}$. Функции

$$f_{\boldsymbol{m}}(\boldsymbol{z}) = \frac{z_1^{m_1} ... z_n^{m_n}}{\sqrt{m_1! ... m_n!}}, \quad m_1, ..., m_n = 0, 1, 2, ...$$

где $\boldsymbol{m} = (m_1, ..., m_n)$ - мультииндекс, образуют ортонормальный базис в $\mathscr{D}_n$. Соответствующие операторы рождения и уничтожения даются формулами

$$a_j^* = z_j, \quad a_j = \frac{\partial}{\partial z_j}, \quad j = 1, ..., n.$$

Гильбертово пространство $\overline{\mathscr{D}}_n$ антиголоморфных функций $f(\overline{\boldsymbol{z}})$ на $\mathbb{C}^n$ определяется скалярным произведением

$$(f, g) = \frac{1}{\pi^n} \int\limits_{\mathbb{C}^n} f(\overline{\boldsymbol{z}})\overline{g(\overline{\boldsymbol{z}})} e^{-|\boldsymbol{z}|^2} d^{2n} z < \infty$$

и операторы рождения и уничтожения даются формулами

$$a_j^* = \bar{z}_j, \quad a_j = \frac{\partial}{\partial \bar{z}_j}, \quad j = 1, ..., n.$$

Когерентные состояния - это $\Phi_{\boldsymbol{v}}(\overline{\boldsymbol{z}}) = e^{\boldsymbol{v}\overline{\boldsymbol{z}}}$, где $\boldsymbol{v}\overline{\boldsymbol{z}} = v_1\bar{z}_1 + \cdots + v_n z_n$, они удовлетворяют воспроизводящему свойству

$$f(\bar{v}) = (f, \Phi_{\boldsymbol{v}}), \quad f \in \overline{\mathscr{D}}_n, \quad v \in \mathbb{C}^n$$

Виковский символ $A(\overline{\boldsymbol{z}}, \boldsymbol{z})$ ограниченного оператора A в $\overline{\mathscr{D}}_n$ определяется как ограничение на подпространство $\boldsymbol{v} = \overline{\boldsymbol{z}}$ целой функции $A(\boldsymbol{v}, \boldsymbol{z})$ от $2n$ переменных $\boldsymbol{v} = (v_1, ..., v_n)$ и $\boldsymbol{z} = (z_1, ..., z_n)$, заданной формулой

$$A(\boldsymbol{v}, \boldsymbol{z}) = e^{-\boldsymbol{v}\boldsymbol{z}} (A\Phi_{\boldsymbol{z}}, \Phi_{\overline{\boldsymbol{v}}})$$

Имеем

$$(Af)(\overline{\boldsymbol{z}}) = \frac{1}{\pi^n} \int\limits_{\mathbb{C}^n} A(\overline{\boldsymbol{z}}, \boldsymbol{v}) f(\overline{\boldsymbol{v}}) e^{-\boldsymbol{v}(\overline{\boldsymbol{v}} - \overline{\boldsymbol{z}})} d^{2n}\boldsymbol{v}, \quad f \in \overline{\mathscr{D}}_n$$

и виковский символ $A(\overline{\boldsymbol{z}}, \boldsymbol{z})$ оператора $A = A_1 A_2$ дается формулой

$$A(\overline{\boldsymbol{z}}, \boldsymbol{z}) = \frac{1}{\pi^n} \int\limits_{\mathbb{C}^n} A_1(\overline{\boldsymbol{z}}, \boldsymbol{v}) A_2(\overline{\boldsymbol{v}}, \boldsymbol{z}) e^{-(\boldsymbol{v} - \boldsymbol{z})(\overline{\boldsymbol{v}} - \overline{\boldsymbol{z}})} d^{2n}\boldsymbol{v}$$

где $A_1(\bar{z}, z)$ и $A_2(\bar{z}, z)$ - виковские символы операторов A_1 и A_2.

Матричный символ $\tilde{A}(\overline{\boldsymbol{z}}, \boldsymbol{z})$ ограниченного оператора A в $\overline{\mathscr{D}}_n$ определяется как ограничение на подпространство $\boldsymbol{v} = \overline{\boldsymbol{z}}$ целой функции $\tilde{A}(\boldsymbol{v}, \boldsymbol{z})$ от $2n$ переменных $\boldsymbol{v} = (v_1, ..., v_n)$ и $\boldsymbol{z} = (z_1, ..., z_n)$, заданной абсолютно сходящимся рядом

$$\tilde{A}(\boldsymbol{v}, \boldsymbol{z}) = \sum_{\boldsymbol{k},\boldsymbol{m}=0}^{\infty} \left(A\bar{f}_{\boldsymbol{k}}, \bar{f}_{\boldsymbol{m}}\right) f_{\boldsymbol{m}}(\boldsymbol{v}) f_{\boldsymbol{k}}(\boldsymbol{z})$$

где $\boldsymbol{k} = (k_1, ..., k_n), \boldsymbol{m} = (m_1, ..., m_n)$ - мультииндексы и $\bar{f}_{\boldsymbol{m}}(\overline{\boldsymbol{z}}) = \overline{f_m(\boldsymbol{z})}$. Матричный и виковский символы ограниченного оператора A связаны формулой

$$\tilde{A}(\boldsymbol{v}, \boldsymbol{z}) = e^{\boldsymbol{v}\boldsymbol{z}} A(\boldsymbol{v}, \boldsymbol{z})$$

ЗАмЕЧАНИЕ. Антиголоморфное представление очень полезно в квантовой механике и особенно в квантовой теории поля, в которой оно называется голоморфным представлением (относительно переменных $\bar{z}$). Слегка злоупотребляя терминологией, в части 2 мы тоже будем называть его голоморфным представлением. ЗАДАЧА 2.15. Найдите явную формулу для унитарного оператора, осуществляющего изоморфизм гильбертовых пространств $\overline{\mathscr{D}}_n \simeq L^2\left(\mathbb{R}^n, d^n q\right)$.

ЗАДАчА 2.16. Докажите, что для ограниченного оператора A функции $A(\boldsymbol{v}, \boldsymbol{z})$ и $\tilde{A}(\boldsymbol{v}, \boldsymbol{z})$ являются целыми функциями от $2n$ переменных.

ЗАДАЧА 2.17. Пусть A - оператор в $\overline{\mathscr{D}}_n$ со следом и $A(\overline{\boldsymbol{z}}, \boldsymbol{z})$ - его виковский символ. Докажите, что

$$\operatorname{Tr} A = \frac{1}{\pi^n} \int\limits_{\mathbb{C}^n} A(\overline{\boldsymbol{z}}, \boldsymbol{z}) e^{-|\boldsymbol{z}|^2} d^{2n}\boldsymbol{z}$$

ЗАДАчА 2.18. Покажите, что виковский символ $A(\bar{z}, z)$ произведения $A = A_l ... A_1$ дается формулой

$$A(\bar{z}, z) = \\ = \frac{1}{\pi^l} \int\limits_{\mathbb{C}^l} A_l\left(\bar{z}, z_{l-1}\right) ... A_1\left(\bar{z}_1, z\right) \exp\left\{\sum_{k=1}^{l} \bar{z}_k \left(z_{k-1} - z_k\right)\right\} d^2 z_1 ... d^2 z_{l-1},$$

где $z_0 = z_l = z, \bar{z}_l = \bar{z}$ и $A_k(\bar{z}, z)$ - виковские символы операторов A_k.

6.4.6 Fermionic Oscillator

(пока только тут теория, потом мб в отдельной записи подробнее буду рассматривать.)

применения фермионного осциллятора (!?!)

(обсудим примеры, зачем он нужен? пока не за чем, поэтому и не занимался им!)
(?? мб в КТП он нужен, там про него что-то еще записано было.)

Фермионный осциллятор используется для описания фермионных полей.
(??)

вкратце описание фермионного осциллятора

грассмановы переменные

Напомним, какими свойствами обладают грассмановы переменные.

Обобщение осциллятора на случай фермионных квантов нетрудно построить в уже изложенном формализме с операторами рождения и уничтожения.

Действительно, предположим, что мы рассматриваем фермион с заданной проекцией спина на ось z и фиксированным набором неспиновых квантовых чисел.

Теперь уже число квантов

$$\hat{n} = \hat{a}^\dagger \hat{a}$$

должно иметь спектр собственных значений

$$n = \{0, 1\}$$

так как согласно принципу запрета Паули в состоянии с фиксированным набором квантовых чисел может находится максимум один квант.

Значит, у фермионного осциллятора базис образуют только два кет-вектора

$$|0\rangle, \quad |1\rangle$$

Для этого необходимо, чтобы действие повышающего оператора на вектор состояния $|1\rangle$ не приводило к возникновению нового состояния:

$$\hat{a}^\dagger |1\rangle = 0$$

Но это есть не что иное, как уравнение на старший вектор. В то же время верно и определение вакуума

$$\hat{a}|0\rangle = 0$$

что, очевидно, можно трактовать как уравнение на младший вектор. В итоге мы имеем квантовую систему с двумя уровнями со старшим и младшим векторами состояний. Такая квантовая систем уже была нами построена-это, по сути, спинор. В ней операторы представляются в базисе (7.7) как матрицы 2×2. Легко провести

следующее отождествление

$$\hat{n} = \frac{1}{2} + \hat{s}_z$$

так как в заданном базисе оператор числа квантов диагонален по построению, как и матрица $\hat{s}_z$ с собственными значениями $\left\{\frac{1}{2}, -\frac{1}{2}\right\}$, откуда

$$\hat{n} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

так что

$$\hat{n} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \hat{n} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$$

и состояния представлены столбцами

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Аналогично повышающий и понижающий операторы становятся операторами рождения и уничтожения:

$$\hat{a}^\dagger = \hat{s}_+, \quad \hat{a} = \hat{s}_-$$

Для них имеет место антикоммутационное соотношение

$$\left\{\hat{a}, \hat{a}^\dagger\right\} = \left\{\left(\hat{s}_x - i\hat{s}_y\right), \left(\hat{s}_x + \mathrm{i}\hat{s}_y\right)\right\} = \left\{\hat{s}_x, \hat{s}_x\right\} + \left\{\hat{s}_y, \hat{s}_y\right\} = 1$$

Значит, для фермионного осциллятора

$$\left\{\hat{a}, \hat{a}^\dagger\right\} = 1$$

сравнение гамильтонианов бозонной и фермионной частиц (???)

Сравним запись для гамильтонианов у бозонной и фермионной частиц.

Именно, у гармонического осциллятора переход от операторов координаты и импульса к операторам рождения и уничтожения квантов приводил к

$$\hat{H}_b = \hbar\omega \frac{1}{2}\left(\hat{a}_b^\dagger \hat{a}_b + \hat{a}_b \hat{a}_b^\dagger\right)$$

и использование стандартного коммутатора $\hat{a}_b \hat{a}_b^\dagger - \hat{a}_b^\dagger \hat{a}_b = 1$ давал

$$\hat{H}_b = \hbar\omega \left(\hat{a}_b^\dagger \hat{a}_b + \frac{1}{2}\right)$$

У фермионных полей возникает вклад вида

$$\hat{H} = \hbar\omega \frac{1}{2}\left(\hat{a}^\dagger \hat{a} - \hat{a}\hat{a}^\dagger\right)$$

и использование стандартного антикоммутатора $\hat{a}\hat{a}^\dagger + \hat{a}^\dagger \hat{a} = 1$ дает

$$\hat{H} = \hbar\omega \left(\hat{a}_b^\dagger \hat{a}_b - \frac{1}{2}\right)$$

Только антикоммутационные соотношения для операторов рождения и уничтожения в этом случае гарантируют, что спектр энергии ограничен снизу и система не проваливается в бесконечность, испуская море энергии.

Интересно отметить, что в случае, если характеристики каждой бозонной моды совпадают с характеристиками такой же фермионной моды, вклад вакуумных между числом бозонных и фермионных вакуумных мод называтот индексом Виттена (имеются примеры даже суперсимметричных теории поля, в которых индекс Виттена отличен от нуля). Симметрия между бозонными и фермионными партнерами называется суперсимметрией.

Возникновение суперсимметрии мы рассмотрим чуть ниже.

А сейчас обратимся к вопросу об описании фермионных мод в терминах когерентных состояний.

Это позволит нам увидеть полную идентичность записи для базиса когерентных состояний у бозонных и фермионных мод с той лишь разницей,

что амплитуды бозонных мод - комплексные числа,

а амплитуды фермионных мод - грассамановы переменные.

Когерентные состояния определяются по-прежнему:

$$\hat{a}|\,\mathrm{th}\rangle = \mathrm{th}\,|\,\mathrm{th}\rangle$$

где необходимо осторожно обращаться с числами нового типа th, свойства которых мы выясним при построении голоморфного представления.

Разложим когерентные состояния по базису.

Для этого рассмотрим

$$\langle 0|\hat{a}|\,\mathrm{th}\rangle = \left(\hat{a}^\dagger|0\rangle\right)^\dagger |\,\mathrm{th}\rangle = \langle 1|\,\mathrm{th}\rangle$$

откуда с учетом условия когерентности (7.15) находим

$$C_1 = \langle 1|\,\mathrm{th}\rangle = \mathrm{th}\langle 0|\,\mathrm{th}\rangle = \mathrm{th}\, C_0$$

Так как разложение включает в себя только два члена,

$$|\,\mathrm{th}\rangle = C_0(|0\rangle + \mathrm{th}\,|1\rangle)$$

Нормировка на единицу дает

$$\langle \mathrm{th}\,|\,\mathrm{th}\rangle = |C_0|^2\,(1 + \bar{\mathrm{th}}\,\mathrm{th}), \quad \bar{\mathrm{th}} = \mathrm{th}^\dagger$$

Кроме того, из соотношений $\left\langle \mathrm{th}\left|\hat{a}^\dagger\hat{a}\right|\mathrm{th}\right\rangle = \bar{\mathrm{th}}\,\mathrm{th}\langle \mathrm{th}\,|\,\mathrm{th}\rangle = \bar{\mathrm{th}}\,\mathrm{th}$, а также

$$\hat{a}|\,\mathrm{th}\rangle = C_0\,\mathrm{th}\,|0\rangle$$

следует, что

$$\left\langle \mathrm{th}\left|\hat{a}^\dagger\hat{a}\right|\mathrm{th}\right\rangle = |C_0|^2\,\bar{\mathrm{th}}\,\mathrm{th} = \bar{\mathrm{th}}\,\mathrm{th}$$

Поэтому в согласии с условием нормировки найдем

$$|C_0|^2\,(1 + \bar{\mathrm{th}}\,\mathrm{th}) = |C_0|^2 + \bar{\mathrm{th}}\,\mathrm{th} = 1$$

Т. е.

$$|C_0|^2 = 1 - \bar{\mathrm{th}}\,\mathrm{th}$$

а также

$$|C_0|^2\,(1 + \bar{\mathrm{th}}\,\mathrm{th}) = (1 - \bar{\mathrm{th}}\,\mathrm{th})(1 + \bar{\mathrm{th}}\,\mathrm{th}) = 1$$

и, следовательно,

$$(\bar{\mathrm{th}}\,\mathrm{th})^2 = 0$$

а значит, и все высшие степени $\bar{\mathrm{th}}\,\mathrm{th}$ обращаются в нуль.

Голоморфное представление (???)

Разложение по базису позволяет построить голоморфное представление в полной аналогии со случаем бозонного осциллятора. Действительно, определим базисные голоморфные функции согласно

$$\langle n|\,\mathrm{th}\rangle = C_0\psi_n^*(\bar{\mathrm{th}}), \quad n = \{0, 1\}$$

Значит,

$$\psi_0(\bar{\mathrm{th}}) = 1, \quad \psi_1(\bar{\mathrm{th}}) = \bar{\mathrm{th}}$$

Отсюда получаем голоморфные представления операторов. Для оператора рождения имеем

$$\hat{a}^\dagger\psi_0(\bar{\mathrm{th}}) = \psi_1(\bar{\mathrm{th}}) \to \hat{a}^\dagger = \bar{\mathrm{th}}$$

Однако, поскольку

$$\hat{a}^\dagger\psi_1(\bar{\mathrm{th}}) = 0$$

получаем необычное свойство числа $\bar{\mathrm{th}}$:

$$\bar{\mathrm{th}}^2 = 0 \leftrightarrow \{\bar{\mathrm{th}}, \bar{\mathrm{th}}\} = 0$$

Взяв эрмитово сопряжение, находим также

$$\{\mathrm{th}, \mathrm{th}\} = 0$$

Собственные значения оператора уничтожения для фермионного осциллятора можно умножать на числа и складывать, так что из соотношений $\mathrm{th}_1^2 = \mathrm{th}_2^2 = 0$ следует, что и собственное число $\mathrm{th}_1 + \mathrm{th}_2$ обладает тем же свойством:

$$(\mathrm{th}_1 + \mathrm{th}_2)^2 = 0 \rightarrow \quad \{\mathrm{th}_1, \mathrm{th}_2\} = \mathrm{th}_1\,\mathrm{th}_2 + \mathrm{th}_2\,\mathrm{th}_1 = 0$$

а значит, перестановка двух собственных чисел происходит со сменой знака. В частности,

$$\mathrm{th}\,\bar{\mathrm{th}} = -\bar{\mathrm{th}}\,\mathrm{th}$$

Для оператора уничтожения

$$\hat{a}\psi_1(\bar{\mathrm{th}}) = \psi_0(\bar{\mathrm{th}}) \rightarrow \hat{a} = \frac{\partial}{\partial\bar{\mathrm{th}}}$$

откуда автоматически

$$\hat{a}\psi_0(\bar{\mathrm{th}}) = 0$$

как и должно быть. Для операторов рождения и уничтожения в голоморфном представлении справедливы антикоммутационные соотношения

$$\left\{\hat{a}, \hat{a}^\dagger\right\} = 1$$

так как на базисных функциях действительно легко вычислить с учетом антикоммутационных соотношений для переменной $\bar{\mathrm{th}}$

$$\left\{\hat{a}, \hat{a}^\dagger\right\}\psi_0(\bar{\mathrm{th}}) = 1 = \psi_0(\bar{\mathrm{th}})$$

и

$$\left\{\hat{a}, \hat{a}^\dagger\right\}\psi_1(\bar{\mathrm{th}}) = \bar{\mathrm{th}} = \psi_1(\bar{\mathrm{th}})$$

С учетом того, что все функции от th и $\bar{\mathrm{th}}$ разлагаются в ряд только до линейных по каждой из переменных членов, можно записать, что

$$1 + \bar{\mathrm{th}}\,\mathrm{th} = e^{\bar{\mathrm{th}}\,\mathrm{th}}$$

откуда

$$|C_0|^2 = e^{-\bar{\mathrm{th}}\,\mathrm{th}}$$

т. е. имеет место прежнее выражение для вклада вакуума в когерентное состояние. Условие полноты когерентных состояний запишем в виде

$$\int \mathrm{d}\bar{\mathrm{th}}\mathrm{d}\,\mathrm{th}\,|\,\mathrm{th}\rangle\langle\mathrm{th}\,|\,| = 1$$

где необходимо определить правила интегрирования так, чтобы выполнялись соотношения ортонормированности базисных векторов. Именно,

$$\int \mathrm{d}\bar{\mathrm{th}}\mathrm{d}\,\mathrm{th}\langle n|\,\mathrm{th}\rangle\langle\mathrm{th}\,|m\rangle = \delta_{nm}, \quad n, m = \{0, 1\}$$

Интеграл можно переписать с помощью голоморфных волновых функций как

$$\int \mathrm{d}\bar{\mathrm{th}}\mathrm{d}\,\mathrm{th}\,e^{-\bar{\mathrm{th}}\,\mathrm{th}}\psi_n^*(\bar{\mathrm{th}})\psi_m(\bar{\mathrm{th}})$$

и в матричном виде получить равенство

$$\int \mathrm{d}\bar{\mathrm{th}}\mathrm{d}\,\mathrm{th}\, e^{-\mathrm{t}\bar{\mathrm{h}}\,\mathrm{th}} \begin{pmatrix} 1 & \mathrm{t}\bar{\mathrm{h}} \\ \mathrm{th} & \mathrm{th}\,\mathrm{t}\bar{\mathrm{h}} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Справедливость этого равенства имеет место, если принять следующие правила интегрирования:

$$\int \mathrm{d}\,\mathrm{th} = \int \mathrm{d}\mathrm{t}\bar{\mathrm{h}} = 0$$
$$\int \mathrm{th}\,\mathrm{d}\,\mathrm{th} = \int \mathrm{t}\bar{\mathrm{h}}\mathrm{d}\mathrm{t}\bar{\mathrm{h}} = 1$$

а также антикоммутативность переменных

$$\{\mathrm{th}, \mathrm{t}\bar{\mathrm{h}}\} = 0$$

и их дифференциалов. Совокупность соотношений антикоммутативности (7.19),(7.20),(7.27) и правила интегрирования (7.25),(17.26) полностью определяют алгебру переменных грассмана или грассмановы преемменные.

голоморфное представление для когерентных состояний фермионов, очевидно, формально повторяет построения в пространстве Баргмана-Фока для бозонных состояний. Стало быть, для вторично квантованного фермионного поля легко записать и решеточную аппроксимацию интеграла Фейнмана в полной аналогии с бозонными полями, используя амплитуды положительно и отрицательно частотных мод в каждом узле решетки импульсного пространства.

Другое о фермионном осцилляторе

примеры применения в КТП

скоро напишу наверное.
вроде бы грассмановы переменные очень много где используются (????)
В вейлевских спинорах это встречается

Сравнение с бозонным осциллятором

6.4.7 Moving oscillator

(порешаю потом задачу)

6.4.8 Oscillator, Moving with $v \approx c$

(тут вопросы про то, как он связан с сокращением длины)

6.4.9 Motion in a Central Field

(мб в другое место вставлю, тут продолб большой, что все еще нет четких методов про это. пока только этот раздел, потом напишу больше и лучше!!!)

Квантовая модель движения в центральном поле по Ландау

(из Ландау скопированы формулы, текст копироваться не хочет)
Одной частице, - аналогично тому, Как это может быть сде.тано

$$\hat{H} = -\frac{\hbar^2}{2m_1}\Delta_1 - \frac{\hbar^2}{2m_2}\Delta_2 + U(r)$$

$$\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1, \quad \mathbf{R} = \frac{m\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}$$

$$\hat{H} = -\frac{\hbar^2}{2\,(m_1 + m_2)}\Delta_R - \frac{\hbar^2}{2m}\Delta + U(r)$$

$$\Delta\psi + \frac{2m}{\hbar^2}[E - U(r)]\psi = 0$$

Воспользовавшись известным выражением для оператора Лапласа $32]

движение в центрально-симметричном поле в сферических координатах, напишем это уравнение в виде

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}\right] + \frac{2m}{\hbar^2}[E - U(r)]\psi = 0$$

если ввести оператор квадрата момента, то мы получим

$$\frac{\hbar^2}{2m}\left[-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{\hat{\mathrm{Im}ath}^2}{r^2}\psi\right] + U(r)\dot{\psi} = E\psi$$

Заданнем значений l и m оп ределяется угловая зависымость ВОл- Hin (32,6) В ВН Ze

$$\psi = R(r)Y_{lm}(\theta, \varphi)$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{l(l+1)}{r^2}R + \frac{2m}{\hbar^2}[E - U(r)]R = 0$$

Это уравнение не содержит вовсе значения $l_2 = m$, что соответст- по направ.тениям момента.

Займемся исследованнем радиальной части волновых функцнй.

Подстановкой

$$R(r) = \frac{\chi(r)}{r}$$

$$\frac{d^2\chi}{dr^2} + \left[\frac{2m}{\hbar^2}(E - U) - \frac{l(l+1)}{r^2}\right]\chi = 0$$

В нуле:

$$\chi(0) = 0$$

В действительности это условне сохраняется (см. $35) также М Для поля, обращающегося при $r \to 0$ В бесконечность.

Уравненне (32,10) по форме совпадает с уравнением ШГредингера дл одномерного движения в поле с потенциальной энергией

$$U_l(r) = U(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$$

равной сумме энергии $U(r)$, и члена

$$\frac{\hbar^2 l(l+1)}{2mr^2} = \frac{\hbar^2\mathbf{2}^2}{2mr^2}$$

Сферические волны по Ландау

(пар 33 ландау)

$$\psi_p = \text{const} \cdot e^{\frac{i}{\hbar}pr}$$

описывает стационарное состояние, в котором свободная частица обладает определенным импульсом p (и энергией $E = p^2/2m$) Рассмотрим теперь такие стационарные состояния свободной Частицы, В Которых она обладает, наряду с энергией, Определенными величиной и проекцией момента.

Вместо энергии нам будет удобно ввести волновой вектор

$$k = \frac{p}{\hbar} = \frac{\sqrt{2mE}}{\hbar}$$

имеет вид

$$\psi_{klm} = R_{kl}(r)Y_{lm}(\theta, \varphi)$$

где радиальная функция определяется уравнением

$$R''_{kl} + \frac{2}{r}R_{kl} + \left[k^2 - \frac{l(l+1)}{r^2}\right]R_{kl} = 0$$

(уравнение (32,8) без $U(r)$). Волновые функции ψ_{klm}, относящиеся К непрерывному (по k) спектру, удовлетворяют условиям нормировки и взаимной ортогональности:

$$\int \psi^*_{k'l'm'}\psi_{klm}dV = \delta_{ll'}\delta_{mm'}\delta\left(\frac{k'-k}{2\pi}\right)$$

(и тут куча деталей, позже их буду писать)

обзор методов рассеяния

падение частицы на центр

(параграф из ландау, а вообще, просто задачка, которую решить можно и писать статью)

движение в кулоновском поле

(параграф из ландау, а вообще, просто задачка, которую решить можно и писать статью)

выводы из нее

обзор применений модели

6.4.10 Angular Momentum Operators

(it was written before, I'll check and then or delete, or move to the previous part)

Теория

В главе 1 (см. пример 1.10 в разделе 1.1.4) мы ввели для классической частицы в $\mathbb{R}^3$ вектор углового момента $\boldsymbol{M}_{\text{c}} = \boldsymbol{x} \times \boldsymbol{p}$ с компонентами

$$M_{\text{c}1} = x_2p_3 - x_3p_2, \quad M_{\text{c}2} = x_3p_1 - x_1p_3, \quad M_{\text{c}3} = x_1p_2 - x_2p_1$$

Согласно примеру 2.1 в разделе 1.2.6 главы 1, у них следующие скобки Пуассона в канонической пуассоновой структуре на $T^*\mathbb{R}^3$:

$$\{M_{c1}, M_{c2}\} = -M_{c3},$$
$$\{M_{c2}, M_{c3}\} = -M_{c1},$$
$$\{M_{c3}, M_{c1}\} = -M_{c2}.$$

Квадрат углового момента $M_c^2 = M_{c1}^2 + M_{c2}^2 + M_{c3}^2$ удовлетворяет условию

$$\{\boldsymbol{M}_c^2, M_{c1}\} = \{\boldsymbol{M}_c^2, M_{c2}\} = \{\boldsymbol{M}_c^2, M_{c3}\} = 0.$$

Если функция Гамильтона

$$H_c(\boldsymbol{p}, \boldsymbol{x}) = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{x})$$

инвариантна при вращениях, $V(\boldsymbol{x}) = V(|\boldsymbol{x}|)$, то компоненты углового момента являются интегралами движения:

$$\{h_c, M_{c1}\} = \{H_c, M_{c2}\} = \{H_c, M_{c3}\} = 0 \quad \text{и} \quad \{H_c, M_c^2\} = 0.$$

Это также можно проверить прямо, используя скобки Пуассона

$$\{M_{cj}, p_k\} = -\varepsilon_{jkl} p_l \quad \text{и} \quad \{M_{cj}, x_k\} = -\varepsilon_{jkl} x_l, \quad i, j, k = 1, 2, 3,$$

где ε_{jkl} - полностью антисимметрический тензор, $\varepsilon_{123} = 1$.

В свою очередь, в квантовой механике компоненты оператора углового момента $\boldsymbol{M} = \boldsymbol{Q} \times \boldsymbol{P}$ определяются формулами

$$M_1 = Q_2 P_3 - Q_3 P_2, \quad M_2 = Q_3 P_1 - Q_1 P_3, \quad M_3 = Q_2 P_3 - Q_3 P_2,$$

где $\boldsymbol{Q} = (Q_1, Q_2, Q_3)$ и $\boldsymbol{P} = (P_1, P_2, P_3)$ - соответственно, операторы координаты и импульса. Поскольку операторы Q_i и P_k коммутируют при $i \neq k$, проблемы упорядочивания при определении операторов квантового углового момента не возникает. Из коммутационных соотношений Гейзенберга следует, что их квантовые скобки устроены также, как и соответствующие скобки Пуассона (3.1):

$$\{M_1, M_2\}_\hbar = -M_3, \quad \{M_2, M_3\}_\hbar = -M_1, \quad \{M_3, M_1\}_\hbar = -M_2.$$

Эквивалентно,

$$[M_1, M_2] = i\hbar M_3, \quad [M_2, M_3] = i\hbar M_1, \quad [M_3, M_1] = i\hbar M_2.$$

Оператор квадрата полного углового момента $\boldsymbol{M}^2 = M_1^2 + M_2^2 + M_3^2$ удовлетворяет уравнению

$$\big[\boldsymbol{M}^2, M_1\big] = \big[\boldsymbol{M}^2, M_2\big] = \big[\boldsymbol{M}^2, M_3\big] = 0.$$

Соответственно, для оператора гамильтониана

$$H = \frac{\boldsymbol{P}^2}{2m} + V(\boldsymbol{Q})$$

со сферически симметрическим потенциалом $V(\boldsymbol{x}) = V(|\boldsymbol{x}|)$ операторы M_1, M_2, M_3, а поэтому и $\boldsymbol{M}^2$, - квантовые интегралы движения:

$$[H, M_1] = [H, M_2] = [H, M_3] = 0 \quad \text{и} \quad \big[H, M^2\big] = 0.$$

Это можно прямо проверить, используя квантовые скобки

$$\{M_j, P_k\}_\hbar = -\varepsilon_{jkl} P_l, \quad \{M_j, Q_k\}_\hbar = -\varepsilon_{jkl} Q_l, \quad j,k,l = 1,2,3,$$

которые устроены так же, как скобки Пуассона (3.2), что следует из коммутационных соотношений Гейзенберга.

В координатном представлении $\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{x})$ операторы углового момента задаются следующими самосопряженными дифференциальными операторами первого порядка:

$$\begin{aligned} M_1 &= i\hbar\left(x_3\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_3}\right), \\ M_2 &= i\hbar\left(x_1\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_1}\right), \\ M_3 &= i\hbar\left(x_2\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_2}\right). \end{aligned}$$

Они обладают свойством, что

$$M_1\psi = M_2\psi = M_3\psi = 0$$

для любой сферически симметричной гладкой функции $\psi(\boldsymbol{x}) = \psi(|\boldsymbol{x}|)$. Иными словами, операторы углового момента действуют только на угловые координаты на $\mathbb{R}^3$. То есть пусть

$$x_1 = r\sin\vartheta\cos\varphi, \quad x_2 = r\sin\vartheta\sin\varphi, \quad x_3 = r\cos\vartheta,$$

где $0 \leqslant \vartheta < \pi, 0 \leqslant \varphi < 2\pi$ - сферические координаты на $\mathbb{R}^3$. Явное вычисление дает

$$\begin{aligned} M_1 &= i\hbar\left(\sin\varphi\frac{\partial}{\partial\vartheta} + \cot\vartheta\cos\varphi\frac{\partial}{\partial\varphi}\right) \\ M_2 &= -i\hbar\left(\cos\varphi\frac{\partial}{\partial\vartheta} - \cot\vartheta\sin\varphi\frac{\partial}{\partial\varphi}\right) \\ M_3 &= -i\hbar\frac{\partial}{\partial\varphi} \end{aligned}$$

Таким образом,

$$M^2 = -\hbar^2\left(\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right)$$

так что оператор $-\frac{1}{\hbar^2}\boldsymbol{M}^2$ - сферическая часть оператора Лапласа на $\mathbb{R}^3$:

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}M^2.$$

6.4.11 SO(3) Representations for the Hydrogen Atom

Теория

Квантовые операторы углового момента связаны с теорией представлений группы вращений SO(3) - группы ортогональных матриц 3×3с определителем 1.SO(3) - компактная группа Ли, изоморфная вещественному проективному пространству $\mathbb{RP}^3$ как гладкое многообразие. Имеется изоморфизм групп Ли $\mathrm{SO}(3) \simeq \mathrm{SU}(2)/\{\pm I\}$, где SU(2) -

группа Ли унитарных матриц 2×2 с определителем 1. Алгебра Ли so(3) группы SO(3) - трехмерная алгебра Ли кососимметрических матриц 3×3 с базисом

$$X_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad X_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad X_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Матрицы X_1, X_2, X_3 порождают соответственно однопараметрические подгруппы SO(3), состоящие из вращений вокруг координатных осей в $\mathbb{R}^3$. Они удовлетворяют коммутационным соотношениям

$$[X_1, X_2] = X_3, \quad [X_2, X_3] = X_1, \quad [X_3, X_1] = X_2,$$

подобным (3.4).

Чтобы установить связь между квантовыми операторами углового момента и теорией представлений SO(3), рассмотрим регулярное представление R группы SO(3) в $\mathscr{H} = L^2(\mathbb{R}^3, d^3\boldsymbol{x})$, определенное формулой

$$(R(g)\psi)(\boldsymbol{x}) = \psi\left(g^{-1}\boldsymbol{x}\right), \quad g \in \mathrm{SO}(3), \psi \in \mathscr{H}$$

Лемма 3.1.

Имеем

$$R\left(e^{u_1X_1+u_2X_2+u_3X_3}\right) = e^{-\frac{i}{\hbar}(u_1M_1+u_2M_2+u_3M_3)}$$

Proof.

Положим $\boldsymbol{uX} = u_1X_1 + u_2X_2 + u_3X_3$ и $\boldsymbol{uM} = u_1M_1 + u_2M_2 + u_3M_3$. Из теоремы Стоуна и прямого вычисления следует, что

$$i\hbar\frac{\partial}{\partial u_j}\bigg|_{u=0} R\left(e^{u\boldsymbol{X}}\right) = M_j, \quad j = 1, 2, 3$$

где самосопряженные операторы M_1, M_2, M_3 даны формулами (3.6)-(3.8). Теперь для фиксированных u_1, u_2, u_3 рассмотрим однопараметрическую группу $U(t) = R\left(e^{tuX}\right)$ унитарных операторов в $\mathscr{H}$. По теореме Стоуна $U(t) = e^{-itA}$, где

$$A = i\frac{d}{dt}\bigg|_{t=0} U(t) = \frac{1}{\hbar}\boldsymbol{uM}$$

ЗАмЕчАНИЕ. Имеем $M_j = i\hbar\rho(X_j)$, где $\rho = dR$ - соответствующее регулярное представление алгебры Ли $\mathfrak{so}(3)$ в $\mathscr{H}$.

Все неприводимые унитарные представления R_l группы Ли SO(3) конечномерны и параметризуются неотрицательными целыми числами $l \geqslant 0$. Соответствующее неприводимое представление $\rho_l = dR_l$ алгебры Ли $\mathfrak{so}(3)$ в $2l+1$ - мерном комплексном векторном пространстве V_l можно явно описать следующим образом. Введем эрмитовы операторы $T_j = i\rho_l(X_j)$, $j = 1, 2, 3$, удовлетворяющие коммутационным соотношениям

$$[T_1, T_2] = iT_3, \quad [T_3, T_1] = iT_2, \quad [T_2, T_3] = iT_1$$

В векторном пространстве V_l есть ортонормированный базис $\{e_{lm}\}_{m=-l}^{m=l}$, такой, что

$$(T_1 - iT_2)\, e_{lm} = -\sqrt{(l+m)(l-m+1)}e_{lm-1}$$
$$(T_1 + iT_2)\, e_{lm} = -\sqrt{(l-m)(l+m+1)}e_{lm+1}$$
$$T_3 e_{lm} = m e_{lm}.$$

В частности, $(T_1 + iT_2)\, e_{ll} = 0$, так что V_l - модуль со старшим весом. Представление ρ_l неприводимо, и по лемме Шура

$$\boldsymbol{T}^2 = l(l+1)I_l$$

где I_l - тождественный оператор в V_l. Это можно также прямо проверить, используя (3.10) − (3.12).

ЗАмЕчАниЕ. Когда l - полуцелое число, т.е. $l \in \frac{1}{2} + \mathbb{Z}_{\geqslant 0}$, и $m = -l, -l+1, ..., l-1, l$, формулы (3.10) − (3.12) все еще определяют неприводимое представление ρ_l старшего веса алгебры Ли $\mathfrak{so}(3)$ размерности $2l+1$, и любое неприводимое n-мерное представление $\mathfrak{so}(3)$ изоморфно представлению $\rho_l cl = \frac{n-1}{2}$. Для полуцелых l представления ρ_l не интегрируемы: они порождают двузначные представления SO(3), так называемые спинорныеб представления. Однако рассматриваемые как представления алгебры Ли $\mathfrak{su}(2) \simeq \mathfrak{so}(3), \rho_l$ соответствуют неприводимым унитарным представлениям группы Ли SU(2). Из теории представлений SU(2) следует, что при $l, l' \in \frac{1}{2}\mathbb{Z}_{\geqslant 0}$

$$V_l \otimes V_{l'} = \bigoplus_{j=|l-l'|}^{l+l'} V_j$$

это так называемое разложение Клебша-Гордона. В физике оно соответствует сложению угловых моментов.

Регулярное представление R группы SO(3) в $\mathscr{H} = L^2(\mathbb{R}^3, d^3x)$ не является неприводимым. Имеем

$$\mathscr{H} = L^2\left(S^2, dn\right) \otimes L^2\left(\mathbb{R}_{>0}, r^2 dr\right)$$

где dn - мера на S^2, индуцированная мерой Лебега на $\mathbb{R}^3$. Группа SO(3) действует вращениями на первом сомножителе тензорного произведения (3.14), тогда как она действует на второй сомножитель как тождественный оператор. Таким образом, задача разложения регулярного представления R сводится к нахождению SO(3)-инвариантных подпространств гильбертова пространства $L^2(S^2, d\boldsymbol{n})$. Итог - разложение в ортогональную сумму

$$L^2\left(S^2, dn\right) = \bigoplus_{l=0}^{\infty} \mathscr{D}_l$$

где $\mathscr{D}_l \simeq V_l$. При этом изоморфизме ортонормированный базис Y_{lm} в $\mathscr{D}_l$, соответствующий базису e_{lm} в V_l, дается нормированными сферическими функциями

$$Y_{lm}(\vartheta, \varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} P_l^m(\cos\vartheta), \quad m = -l, ..., l$$

где $P_l^m(x)$ - нормированные присоединенные полиномы Лежандра,

$P_l^m(x) = (-1)^m \sqrt{\frac{(l+m)!}{(l-m)!}} \sqrt{\frac{2l+1}{2}} \frac{1}{2^l l!} \left(1-x^2\right)^{-\frac{m}{2}} \frac{d^{l-m}}{dx^{l-m}} \left(x^2-1\right)^l, .|x| < 1$

Самосопряженный оператор M^2 в гильбертовом пространстве $L^2(S^2, d\boldsymbol{n})$ имеет чисто точечный спектр, состоящий из собственных значений $\hbar^2 l(l+1)$ кратностей $2l+1, l = 0, 1, 2, ...$, и разложение (3.15) дает разложение по его собственным функциям: для любого $\psi \in L^2(S^2, d\boldsymbol{n})$

$$\psi = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} C_{lm} Y_{lm}, \quad \text{где } C_{lm} = \int_0^{2\pi} \int_0^{\pi} \psi(\vartheta, \varphi) \overline{Y_{lm}(\vartheta, \varphi)} \sin\vartheta d\vartheta d\varphi$$

ЗАдАЧА 3.1. Докажите все результаты этого раздела. (Указание: см. литературу к этой главе.)

6.5 Harmonic Oscillator: Advanced Ideas

6.5.1 Overview of Applications of Harmonic Oscillator

(surprisingly, there are a lot of applications. I'll discuss them here)

6.5.2 Discrete Spectrum in a Central Field

Теория по Тахтаджаяну

Атом водорода описывается дальнодействующим потенциалом

$$V(\boldsymbol{r}) = -\frac{\alpha}{r}$$

кулоновским потенциалом, где $\alpha > 0$[3]. Соответствующая задача о собственных значениях для оператора Шрёдингера с кулоновским потенциалом называется кулоновской задачей. Здесь мы представим ее точное решения, используя так называемые кулоновские единицы $\hbar = 1, \mu = 1$, и $\alpha = 1$[4].

Чтобы определить дискретный спектр, удобно положить $2E = -\varkappa^2 < 0$, так что уравнение на собственные значения (4.10) превращается в

$$f_l'' + \left(\frac{2}{r} - \frac{l(l+1)}{r^2} - \varkappa^2\right) f_l = 0.$$

Асимптотики (4.12) - (4.13) для короткодействующих потенциалов наводят на мысль, что для дальнодействующего кулоновского потенциала можно искать решение с интегрируемым квадратом в следующем виде:

$$f_l(r) = r^{l+1} e^{-\varkappa r} \Lambda(r).$$

Подставив это в (5.1), получаем уравнение

$$\Lambda_l'' + \left(\frac{2(l+1)}{r} - 2\varkappa\right)\Lambda_l' + \left(\frac{2}{r} - \frac{2\varkappa(l+1)}{r}\right)\Lambda_l = 0,$$

которое можно решить с помощью степенного ряда

$$\Lambda_l(r) = \sum_{k=0}^{\infty} a_k r^k$$

Подстановка этого степенного ряда в (5.2) дает следующее рекуррентное соотношение для коэффициентов a_k:

$$a_{k+1} = \frac{2\varkappa(k+l+1) - 2}{(k+1)(k+2l+2)} a_k, \quad k = 1, 2, ...,$$

[3] Для атома водорода $\alpha = e^2$, где e - заряд электрона. Случай $\alpha = Ze^2$, где $Z = 2, 3, ...$, соответствует ионам водорода.

[4] Когда $\alpha = e^2$, кулоновские единицы совпадают с атомными единицами. где $a_0 \neq 0$. Степенной ряд (5.3) сходится при всех $r > 0$ по признаку сходимости Даламбера. Когда $\varkappa > 0$ таково, что $a_k \neq 0$ для любого k, имеем

$$\lim_{k\to\infty}\frac{(k+1)a_{k+1}}{a_k}=2\varkappa.$$

Таким образом, для любого $\varepsilon>0$ существует N, такое, что при $k>N$ все a_k одного знака, скажем $a_k>0$, и

$$\frac{a_{k+1}}{a_k}\geqslant\frac{2\varkappa-\varepsilon}{k+1}$$

Тогда при $k>N$ получаем

$$a_k\geqslant C\frac{(2\varkappa-\varepsilon)^k}{k!}$$

с некоторой константой $C>0$ (зависящей от ε), и поскольку для фиксированного N сумма первых N членов в (5.3) растет как r^N при $r\to\infty$, для достаточно большого r получаем [5]

$$\Lambda_l(r)\geqslant Ce^{(2\varkappa-\varepsilon)r}-C_1r^N>C_2e^{(2\varkappa-\varepsilon)r}.$$

Этим доказывается, что для таких значений $\varkappa$ функция $f_l(r)$ не интегрируема с квадратом на $(0,\infty)$. Однако для особых значений

$$\varkappa=\varkappa_{kl}=\frac{1}{k+l+1}$$

степенной ряд (5.3) обрывается: $\Lambda_l(r)$ превращается в многочлен $\Lambda_{kl}(r)$ порядка k и $f_{kl}(r)=r^{l+1}e^{-\varkappa_{kl}r}\Lambda_{kl}(r)\in L^2(0,\infty)$. Положив $n=k+l+1$, получаем явную формулу для собственных значений

$$E_n=-\frac{1}{2n^2},\quad n=1,2,...$$

Для фиксированного n целое число l изменяется от 0 до $n-1$, и для каждого l имеется $2l+1$ ортогональных собственных функций $\frac{f_{kl}(r)}{r}Y_{lm}(\boldsymbol{n})$ с собственным значением E_n. Таким образом, полная кратность собственного значения E_n равна

$$\sum_{l=0}^{n-1}(2l+1)=n^2.$$

[5] Можно показать, что $\Lambda_l(r)=Ce^{2\varkappa r}(1+o(1))$ при $r\to\infty$. Собственные функции $f_{kl}(r)$ радиального уравнения Шрёдингера (5.1), соответствующие собственному значению E_n, можно выразить в терминах классических многочленов Лагерра. А именно: при $\varkappa=\frac{1}{n}$ подстановка $x=\frac{2r}{n}$ сводит дифференциальное уравнение (5.2) к

$$xQ''+(p+1-x)Q'+kQ=0,$$

где $p=2l+1$ и $Q(x)=\Lambda_l(r)$. Это - дифференциальное уравнение, которому удовлетворяют обобщенные многочлены Лагерра $Q_k^p(x)$, определенные формулой

$$Q_k^p(x)=e^xx^{-p}\frac{d^k}{dx^k}\left(e^{-x}x^{k+p}\right),$$

это многочлены степени k со старшим коэффициентом $(-1)^k$, у которых имеется k нулей в промежутке $(0,\infty)$. Для каждого p обобщенные многочлены Лагерра $\{Q_k^p(x)\}_{k=0}^{\infty}$ - это ортогональные по мере $e^{-x}x^pdx$ многочлены на $(0,\infty)$ со свойством

$$\int_0^\infty e^{-x}x^{p+1}Q_k^p(x)^2dx = k!(k+p)!(2k+p+1).$$

Ортонормированные собственные функции оператора Шрёдингера H для атома водорода, соответствующие собственному значению E_n, имеют вид

$$\psi_{klm}(\boldsymbol{q}) = \frac{2}{n^2}\frac{1}{\sqrt{k!(n+l)!}}\left(\frac{2r}{n}\right)^l e^{-\frac{r}{n}}Q_k^{2l+1}\left(\frac{2r}{n}\right)Y_{lm}(\boldsymbol{n})$$

где $n = k+l+1, l = 0,...,n-1$, и $m = -l,...,l$.

ЗАМЕчАниЕ. Возвращаясь к физическим единицам $\alpha = e^2$, где e - заряд электрона, получаем для уровней энергии атома водорода

$$E_n = -\frac{\mu e^4}{2n^2\hbar^2}$$

где μ - приведенная масса электрона и ядра. В частности, энергия основного состояния $-E_1 = -13,6\text{eV}$; ее абсолютная величина - это энергия

[6] Также используются многочлены $L_n^m(x) = (-1)^m\frac{n!}{(n-m)!}Q_{n-m}^m(x)$. ионизачии - энергия, необходимая, чтобы удалить электрон из атома водорода. Используя формулу Бора для частот спектральных линий

$$\hbar\omega_{mn} = E_n - E_m$$

получаем для атома водорода

$$\omega_{nm} = \frac{\mu e^4}{2\hbar^3}\left(\frac{1}{n^2}-\frac{1}{m^2}\right), \quad n < m.$$

При $n = 1$ и $m = 2,3,...$ получаем классическую серию Лаймана, $n = 2$ и значения $m = 3,4,...$ дают серию Балмера, тогда как $n = 3$ и $m = 4,5,...$ - серию Пашена. Эти серии спектральных линий были открыты экспериментально задолго до того, как была сформулирована квантовая механика.

ЗАМЕЧАНИЕ. Уровни энергии атома водорода можно также определить из правил квантования Бора-Вильсона-Зоммерфельда. А именно: в сферических координатах (r,ϑ,φ) на $\mathbb{R}^3$ лагранжиан задачи Кеплера принимает вид (см. раздел 1.1.6 главы 1)

$$L = \frac{1}{2}\mu\left(\dot r^2 + r^2\dot\vartheta^2 + r^2\sin^2\vartheta\dot\varphi^2\right) + \frac{\alpha}{r},$$

и соответствующие обобщенные импульсы - это

$$p_r = \mu\dot r, \quad p_\vartheta = \mu r^2\dot\vartheta, \quad p_\varphi = \mu r^2\sin^2\vartheta\dot\varphi.$$

Условия квантования БВЗ

$$\oint p_r dr = 2\pi\hbar\left(k+\frac{1}{2}\right)$$
$$\oint p_\vartheta d\vartheta = 2\pi\left(l-m+\frac{1}{2}\right)$$
$$\oint p_\varphi d\varphi = 2\pi\hbar m$$

в которых интегрирование ведется по замкнутой орбите задачи Кеплера с энергией $E < 0$, точно определяют уровни энергии $E_n, n = k+l+1$.

Действительно, имеем $p_\varphi = M_{c3}$, где $\boldsymbol{M}_c = (M_{c1}, M_{c2}, M_{c3})$ - классический угловой момент. Он постоянен на орбите, так что уравнение (5.7) определяет собственные значения оператора M_3 (см. раздел 3.3.2). Для вычисления $\oint p_\vartheta d\vartheta$ воспользуемся полярными координатами (r, χ) в плоскости орбиты P (см. раздел 1.1.6 главы 1). Поскольку $\dot\chi^2 = \dot\vartheta^2 + \sin^2\vartheta\dot\varphi^2$, на орбите получаем $p_\chi d\chi = p_\vartheta d\vartheta + p_\varphi d\varphi$, где $p_\chi = \mu r^2\dot\chi = |\boldsymbol{M}_c|$. Условие (5.6) теперь следует из равенства

$$\oint p_\chi d\chi = 2\pi\,|\boldsymbol{M}_c| = 2\pi\hbar\left(l + \frac{1}{2}\right)$$

то есть из правила квантования квадрата полного углового момента [7]. Наконец, чтобы вычислить $\oint p_r dr$, воспользуемся уравнениями (1.7) и (1.11) из раздела 1.1.6 главы 1 и получим, что

$$p_r dr = \mu\dot r dr = \mu\frac{dr}{d\chi}\dot\chi dr = \frac{|\boldsymbol{M}_c|}{r^2}\left(\frac{dr}{d\chi}\right)^2 d\chi = p_\chi\frac{e^2\sin^2\chi}{(1+e\cos\chi)^2}d\chi$$

где $0 < e < 1$ - эксцентриситет орбиты. Имеем

$$\oint p_r dr = p_\chi\int_0^{2\pi}\frac{e^2\sin^2\chi}{(1+e\cos\chi)^2}d\chi = 2\pi p_\chi\left(\frac{1}{\sqrt{1-e^2}} - 1\right),$$

что может быть показано с помощью подстановки $z = e^{i\chi}$ и теоремы Коши о вычетах [8]. Из уравнения (1.12) в разделе 1.1.6 главы 1 следует, что

$$\sqrt{1-e^2} = \frac{|\boldsymbol{M}_c|\,\sqrt{2|E|}}{\alpha\sqrt{\mu}}$$

и из (5.5) и (5.8) получаем

$$|E| = -E_n = \frac{\mu\alpha^2}{2n^2\hbar^2}, \quad n = k + l + 1.$$

[7] Это равенство дает квантованные значения $\hbar^2\left(l+\frac{1}{2}\right)^2$, при больших l хорошо согласующиеся с собственными значениями $\hbar^2 l(l+1)$ оператора M^2.

[8] Этот интеграл был вычислен Зоммерфельдом в 1916 г.

6.5.3 Continuous Spectrum in a Central Field

Теория по Тахтаджаяну

Положим $2E = k^2$, где $k > 0$, и рассмотрим уравнение

$$f_l'' + \left(\frac{2}{r} - \frac{l(l+1)}{r^2} + k^2\right) f_l = 0.$$

Подстановкой

$$f_l(r) = r^{l+1}e^{-ikr}F_l(r)$$

уравнение (5.9) сводится к

$$F_l'' + \left(\frac{2(l+1)}{r} - 2ik\right)F_l' + \left(\frac{2}{r} - \frac{2ik(l+1)}{r}\right)F_l = 0.$$

Решение уравнения (5.10), удовлетворяющее условию $F_l(0) = 1$, можно в явном виде записать как

$$F_l(r) = F(l+1+i\lambda, 2l+2, 2ikr), \quad \lambda = \frac{1}{k},$$

где $F(\alpha,\gamma,z)$ - вырожденная гипергеометрическая функция, определенная абсолютно сходящимся рядом

$$F(\alpha,\gamma,z) = \sum_{n=0}^{\infty} \frac{\Gamma(\alpha+n)\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma+n)} \frac{z^n}{n!}$$

для всех α и $\gamma \neq 0, -1, -2, ...$ Вырожденная гипергеометрическая функция является целой функцией от переменной z и удовлетворяет дифференциальному уравнению

$$zF'' + (\gamma - z)F' - \alpha F = 0.$$

При $\alpha = -k$ и $\gamma = p+1$, где $k, p = 0, 1, 2, ...$, вырожденная гипергеометрическая функция сводится к обобщенным многочленам Лагерра:

$$Q_k^p(x) = \frac{(k+p)!}{p!} F(-k, p+1, x),$$

рассмотренным в предыдущем разделе. При $\operatorname{Re}\gamma > \operatorname{Re}\alpha > 0$ функция $F(\alpha,\gamma,z)$ допускает интегральное представление

$$F(\alpha,\gamma,z) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma-\alpha)} \int_0^1 t^{\alpha-1}(1-t)^{\gamma-\alpha-1} e^{zt} dt$$

получаемое по методу Лапласа. Вырожденная гипергеометрическая функция удовлетворяет функциональному уравнению

$$F(\alpha,\gamma,z) = e^z F(\gamma-\alpha, \gamma, -z)$$

и имеет следующую асимптотику при $z \to \infty$:

$$F(\alpha,\gamma,z) = \frac{\Gamma(\gamma)}{\Gamma(\gamma-\alpha)}(-z)^{-\alpha}\left(1 + O\left(z^{-1}\right)\right) + \frac{\Gamma(\gamma)}{\Gamma(\alpha)} e^z z^{\alpha-\gamma}\left(1 + O\left(z^{-1}\right)\right).$$

Из (5.12) следует, что функция $f_l(r) = r^{l+1}e^{-ikr}F(l+1+i\lambda, 2l+ \ +2, 2ikr)$ вещественнозначна, а из (5.13) следует, что функция

$$f_{El}(r) = \frac{(2k)^{l+1}}{\sqrt{2\pi}(2l+1)!} e^{\frac{\pi}{2k}} |\Gamma(l+1-i\lambda)| f_l(r)$$

имеет следующую асимптотику при $r \to \infty$:

$$f_{El}(r) = \sqrt{\frac{2}{\pi}} \sin\left(kr + \lambda \log 2kr - \frac{l\pi}{2} + \delta_l\right) + o(1),$$

где

$$\delta_l(k) = \arg\Gamma(l+1-i\lambda), \quad \lambda = \frac{1}{k} = \frac{1}{\sqrt{2E}}$$

фазовый сдвиг. Частичная S-матрица для кулоновской задачи - это

$$S_l(k) = e^{2i\delta_l(k)} = \frac{\Gamma(l+1-i\lambda)}{\Gamma(l+1+i\lambda)}.$$

Она допускает мероморфное продолжение в верхнюю полуплоскость $\operatorname{Im} k > 0$ и имеет простые полюса в точках $k = i\varkappa_{jl}$, соответствующих собственным значениям E_{kl}

радиального оператора Шрёдингера H_l. Радиальные собственные функции непрерывного спектра (5.14) удовлетворяют условию нормировки (4.15).

ЗАМЕЧАНИЕ. Поучительно сравнить асимптотику (5.15) для кулоновского потенциала, являющегося дальнодействующим, с соответствующей формулой (4.16) для общего короткодействующего потенциала. Дальнодействующая природа кулоновского взаимодействия проявляется в добавочном логарифмическом члене $\lambda \log 2kr$ в (5.15).

Теорема о разложении по собственным функциям для оператора Шрёдингера H атома водорода имеет такой же вид, как и в разделе 3.4.3: собственные функции $\psi_{klm}(\boldsymbol{x})$ даются формулой (5.4), где $k = 0, 1, ..., N_l = \infty$, а собственные функции непрерывного спектра даются формулой

$$\psi_{Elm}(\boldsymbol{x}) = \frac{f_{El}(r)}{r} Y_{lm}(\boldsymbol{n}), \quad l = 0, 1, ..., \quad m = -l, ..., l$$

6.5.4 Hidden SO(4) Symmetry

Теория в центральном поле по Тахтаджаяну

Как мы видели в разделе 1.1.6 главы 1, у классической системы с функцией Гамильтона

$$H_{\mathrm{c}}(\boldsymbol{p}, \boldsymbol{x}) = \frac{p^2}{2m} - \frac{\alpha}{r}$$

вдобавок к угловому моменту M_{c} есть три добавочных интеграла движения, которые даются вектором Лапласа - Рунге - Ленца

$$\boldsymbol{W}_{\mathrm{c}} = \frac{\boldsymbol{p}}{m} \times M_{\mathrm{c}} - \frac{\alpha \boldsymbol{x}}{\boldsymbol{r}}$$

Согласно примеру 2.2 из раздела 1.2.6 главы 1, интегралы M_{c} и W_{c} для задачи Кеплера имеют скобки Пуассона:

$$\{M_{\mathrm{c}j}, M_{\mathrm{ck}}\} = -\varepsilon_{jkl} M_{\mathrm{cl}}, \quad \{W_{\mathrm{c}j}, M_{\mathrm{ck}}\} = -\varepsilon_{jkl} W_{\mathrm{cl}},$$
$$\{W_{\mathrm{c}j}, W_{\mathrm{ck}}\} = 2H_{\mathrm{c}} \varepsilon_{jkl} M_{\mathrm{cl}},$$

где $j, k, l = 1, 2, 3$ и $\varepsilon_{123} = 1$.

Квантовая задача Кеплера - это кулоновская задача. В координатном представлении $\mathscr{H} = L^2(\mathbb{R}^3, d^3x)$ ее гамильтониан - это

$$H = \frac{\boldsymbol{P}^2}{2} - \frac{\alpha}{r}$$

где $r = |\boldsymbol{x}|$, и мы положили $m = 1$. Квантовый вектор Лапласа-РунгеЛенца - оператор Лапласа-Рунге - Ленца W - определяется формулой

$$\boldsymbol{W} = \frac{1}{2}(\boldsymbol{P} \times \boldsymbol{M} - \boldsymbol{M} \times \boldsymbol{P}) - \frac{\alpha \boldsymbol{Q}}{r}$$

или Покомпонентно -

$$W_j = \frac{1}{2} \varepsilon_{jkl} (P_k M_l + M_l P_k) - \frac{\alpha Q_j}{r}, \quad j = 1, 2, 3$$

Здесь Q_i - операторы умножения на x_i, и все время подразумевается суммирование по повторяющимся индексам 1, 2, 3. В силу коммутационных соотношений (3.5) имеем также

$$W = P \times M - \frac{\alpha Q}{r} - i\hbar P = -M \times P - \frac{\alpha Q}{r} + i\hbar P$$

где слагаемое $i\hbar \boldsymbol{P}$ играет роль «квантовой поправки». Следующий результат выявляет скрытую симметрию кулоновской задачи.

Предложение 5.1.

Оператор Шрёдингера H атома водорода имеет шесть квантовых интегралов движения $\boldsymbol{MW}$,

$$[H, M_i] = [H, W_i] = 0, \quad i = 1, 2, 3$$

удовлетворяющих условиям $\boldsymbol{W} \cdot \boldsymbol{M} = \boldsymbol{M} \cdot \boldsymbol{W} = 0$ и

$$\boldsymbol{W}^2 = \alpha^2 + 2HM^2 + 2\hbar^2 H$$

Кроме того, самосопряженные операторы $\boldsymbol{M}$ и $\boldsymbol{W}$ уовлетворяют следуючим коммутачионным соотношениям:
$[M_j, M_k] = i\hbar\varepsilon_{jkl}M_l, \quad [W_j, M_k] = i\hbar\varepsilon_{jkl}W_l, \quad [W_j, W_k] = -2i\hbar\varepsilon_{jkl}M_l H$

Proof.

Мы знаем, что $[H, M_j] = 0$. Чтобы доказать, что W_j - квантовые интегралы движения, сперва вычислим $\left[\boldsymbol{P}^2, \frac{Q_j}{r}\right]$. Из коммутационных соотношений Гейзенберга следует, что

$$\left[P_j, \frac{1}{r}\right] = i\hbar\frac{Q_j}{r^3}$$

так что, используя правила Лейбница и соотношения $r^2 = x_1^2 + x_2^3 + x_3^2$, $[M_l, r] = 0$ и $Q_j P_k - Q_k P_j = \varepsilon_{jkl}M_l$, получаем

$$\left[\boldsymbol{P}^2, \frac{Q_j}{r}\right] = 2i\hbar\frac{Q_j}{r^3} + 2i\hbar\varepsilon_{jkl}\frac{Q_k}{r^3}M_l$$

Теперь, воспользовавшись первым уравнением в (5.17) и уравнением (5.19), получаем

$$\begin{aligned}[H, W_j] &= \left[\frac{\boldsymbol{P}^2}{2} - \frac{\alpha}{r}, \varepsilon_{jkl}P_k M_l - \frac{\alpha Q_j}{r} - i\hbar P_j\right] = \\ &= -i\alpha\hbar\frac{Q_j}{r^3} - i\alpha\hbar\varepsilon_{jkl}\frac{Q_k}{r^3}M_l + i\alpha\hbar\varepsilon_{jkl}\frac{Q_k}{r^3}M_l + i\alpha\hbar\frac{Q_j}{q^3} = 0\end{aligned}$$

Легко доказать соотношение $\boldsymbol{W} \cdot \boldsymbol{M} = W_1M_1 + W_2M_2 + W_3M_3 = 0$. Действительно, из определения M и коммутативности P_k и Q_l при $k \neq l$ следует, что

$$\boldsymbol{M} \cdot \boldsymbol{P} = \boldsymbol{P} \cdot \boldsymbol{M} = \boldsymbol{M} \cdot \boldsymbol{Q} = \boldsymbol{Q} \cdot \boldsymbol{M} = 0$$

и, используя первое уравнение в (5.17) и коммутационные соотношения для компонент углового момента, немедленно получаем, что $\boldsymbol{W} \cdot \boldsymbol{M} = 0$. Чтобы доказать, что $M \cdot W = 0$, надо воспользоваться вторым уравнением в (5.17).

Проверка условия (5.18) требует большей работы. Имеем

$$\begin{aligned}\boldsymbol{W}^2 = W_j W_j = \\ = \left(\varepsilon_{jkl} M_l P_k - \frac{\alpha Q_j}{r} + i\hbar P_j\right)\left(\varepsilon_{jmn} P_m M_n - \frac{\alpha Q_j}{r} - i\hbar P_j\right) = \\ = \varepsilon_{jkl}\left(\varepsilon_{jmn} M_l P_k P_m M_n - \alpha M_l P_k \frac{Q_j}{r} - i\hbar M_l P_k P_j\right) - \\ - \alpha\varepsilon_{jmn}\frac{Q_j}{q} P_m M_n + \alpha^2 \frac{Q_j Q_j}{r^2} + i\alpha\hbar\frac{Q_j}{r} P_j + i\hbar\varepsilon_{jmn} P_j P_m M_n - \\ - i\alpha\hbar P_j \frac{Q_j}{r} + \hbar^2 P_j P_j = \\ = \alpha^2 I + \hbar^2 P^2 + \varepsilon_{jkl}\varepsilon_{jmn} M_l P_k P_m M_n - \\ - \alpha\varepsilon_{jkl}\left(M_l P_k \frac{Q_j}{q} + \frac{Q_j}{r} P_k M_l\right) - i\alpha\hbar\left[P_j, \frac{Q_j}{r}\right].\end{aligned}$$

Поскольку операторы M_j и P_j коммутируют, тождество $(\boldsymbol{a}\times\boldsymbol{b})^2 = \boldsymbol{a}^2\boldsymbol{b}^2$ - $-(a\cdot b)^2$ по-прежнему применимо, и мы получаем, что

$\varepsilon_{jkl}\varepsilon_{jmn} M_l P_k P_m M_n = -(\boldsymbol{M}\times\boldsymbol{P})\cdot(\boldsymbol{P}\times\boldsymbol{M}) = \boldsymbol{M}^2\boldsymbol{P}^2 - (\boldsymbol{M}\cdot\boldsymbol{P})^2 = \boldsymbol{M}^2\boldsymbol{P}^2$. Используя (5.19), легко находим (суммирование по повторяющимся индексам), что

$$\left[P_j, \frac{Q_j}{r}\right] = i\hbar\left(-\frac{3}{r} + \frac{r^2}{r^3}\right) = -\frac{2i\hbar}{r}$$

Поскольку $[\boldsymbol{M}^2, r] = 0$, из равенства $\boldsymbol{M} = \boldsymbol{Q}\times\boldsymbol{P}$ следует, что

$$\varepsilon_{jkl}\left(M_l P_k \frac{Q_j}{r} + \frac{Q_j}{r} P_k M_l\right) = M^2\frac{1}{r} + \frac{1}{r}M^2 = \frac{2M^2}{r}$$

Собирая все вместе, получаем (5.18).

Нетрудно также установить коммутационные соотношения между M_j и W_k. Используя (3.5) и свойства ε_{jkl}, получаем

$$\begin{aligned}[M_j, W_k] = \left[M_j, \varepsilon_{kmn} P_m M_n - \frac{\alpha Q_k}{r} - i\hbar P_k\right] = \\ = i\hbar\left(\varepsilon_{jmp}\varepsilon_{kmn} P_p M_n + \varepsilon_{jnp}\varepsilon_{kmn} P_m M_p\right) - i\hbar\varepsilon_{jkl}\left(\frac{\alpha Q_l}{r} + i\hbar P_l\right) = \\ = i\hbar\left(P_j M_k - M_k P_j\right) - i\hbar\varepsilon_{jkl}\left(\frac{\alpha r_l}{r} + i\hbar P_l\right) = i\hbar\varepsilon_{jkl} W_l\end{aligned}$$

Наконец, чтобы установить коммутационные соотношения между компонентами W, воспользуемся представлениями

$$\boldsymbol{W} = \boldsymbol{Q}\boldsymbol{P}^2 - \boldsymbol{P}(\boldsymbol{Q}\cdot\boldsymbol{P}) - \frac{\alpha\boldsymbol{Q}}{r} = \boldsymbol{P}^2\boldsymbol{Q} - (\boldsymbol{P}\cdot\boldsymbol{Q})\boldsymbol{P} - \frac{\alpha\boldsymbol{Q}}{r}$$

Первая формула в (5.20) следует из первой формулы в (5.17), если воспользоваться соотношениями

$$\begin{aligned}\varepsilon_{jkl} P_k M_l = \varepsilon_{jkl}\varepsilon_{lmn} P_k Q_m P_l = \varepsilon_{jkl}\left(\varepsilon_{ljk} P_k Q_j P_k + \varepsilon_{lkj} P_k Q_k P_j\right) = \\ = P_k\left(P_k Q_j - P_j Q_k\right) = Q_j\boldsymbol{P}^2 - P_j(\boldsymbol{P}\cdot\boldsymbol{Q}) - 2i\hbar P_j\end{aligned}$$

и соотношением $\boldsymbol{P}\cdot\boldsymbol{Q} = \boldsymbol{Q}\cdot\boldsymbol{P} - 3i\hbar I$. Вторая формула в (5.20) следует из первой в силу коммутационных соотношений Гейзенберга. Дальше имеем

$$\varepsilon_{jkl}\,[W_k, W_l] = 2\varepsilon_{jmn} W_m W_n =$$
$$= 2\varepsilon_{jmn}\left(\boldsymbol{P}^2 Q_m - (\boldsymbol{P}\cdot\boldsymbol{Q})P_m - \frac{\alpha Q_m}{r}\right)\left(Q_n \boldsymbol{P}^2 - P_n(\boldsymbol{Q}\cdot\boldsymbol{P}) - \frac{\alpha Q_n}{r}\right) =$$
$$= 2M_j\left(-\boldsymbol{P}^2(\boldsymbol{Q}\cdot\boldsymbol{P}) + (\boldsymbol{P}\cdot\boldsymbol{Q})\boldsymbol{P}^2 + \frac{\alpha}{r}(\boldsymbol{Q}\cdot\boldsymbol{P}) - (\boldsymbol{P}\cdot\boldsymbol{Q})\frac{\alpha}{r}\right) =$$
$$= -2i\hbar M_j\left(\boldsymbol{P}^2 - \frac{2\alpha}{r}\right) = -4i\hbar M_j H$$

где были использованы равенства $[\boldsymbol{M}, \boldsymbol{P}\cdot\boldsymbol{Q}] = 0$ и $\left[\boldsymbol{P}\cdot\boldsymbol{Q}, \frac{1}{r}\right] = \frac{i\hbar}{r}$. Это доказывает, что $[W_k, W_l] = -2i\hbar\varepsilon_{jkl} M_j H$.

Пусть $\mathscr{H}_0 = \mathrm{P}_H(-\infty, 0)\mathscr{H}$, где P_H - проекторная мера для оператора Шрёдингера H. Поскольку самосопряженные операторы $\boldsymbol{M}$ и $\boldsymbol{W}$ коммутируют с H, подпространство $\mathscr{H}_0$ - инвариантное подпространство для этих операторов. Оператор Шрёдингера H неотрицателен на $\mathscr{H}_0$, так что на этом пространстве корректно определен оператор $(-2H)^{-1/2}$. Далее, на $\mathscr{H}_0$ положим

$$\boldsymbol{J}^{(\pm)} = \frac{1}{2}\left(\boldsymbol{M} \pm (-2H)^{-1/2}\boldsymbol{W}\right)$$

Из предложения 5.1 следует, что самосопряженные операторы $J_j^{(\pm)}$на $\mathscr{H}_0$ удовлетворяют коммутационным соотношениям

$$\left[J_j^{(\pm)}, J_k^{(\pm)}\right] = i\hbar\varepsilon_{jkl} J_l^{(\pm)}, \quad \left[J_j^{(+)}, J_k^{(-)}\right] = 0$$

и

$$\left(J^{(+)}\right)^2 = \left(J^{(-)}\right)^2 = -\frac{1}{4}\left(\hbar^2 I + \frac{\alpha^2}{2H}\right).$$

Уравнения (5.21) - это коммутационные соотношения для образующих алгебры Ли $\mathfrak{so}(4)$, что соответствует изоморфизму алгебр Ли $\mathfrak{so}(4) \simeq \mathfrak{so}(3) \oplus \mathfrak{so}(3)$ и чем демонстрируется скрытая SO(4) симметрия кулоновской задачи! Вместе с (5.22) они позволяют найти уровни энергии чисто алгебраически.

А именно: собственные значения операторов $\left(J^{(+)}\right)^2$ и $\left(J^{(-)}\right)^2$ - это соответственно $\hbar^2 l_1\,(l_1+1)$ и $\hbar^2 l_2\,(l_2+1)$, и из (5.22) следует, что $l_1 = l_2 = l$, так что соответствующее собственное значение H - это

$$E_n = -\frac{\alpha^2}{2\hbar^2 n^2}, \quad n = 2l+1$$

Предполагая, что

$$\mathscr{H}_0 \simeq \bigoplus_{l\in\frac{1}{2}\mathbb{Z}_{\geqslant 0}} V_l \otimes V_l,$$

где суммирование происходит по всем неотрицательным целым и полуцелым значениям l, получаем из разложения Клебша-Гордона (3.13), что кратность собственного значения E_n - это

$$\dim V_l \otimes V_l = \sum_{j=0}^{2l}(2j+1) = (2l+1)^2 = n^2$$

Для доказательства ортогонального разложения (5.23) надо рассмотреть уравнение Шрёдингера для атома водорода в импульсном представлении. Используя сферические координаты в $\mathbb{R}^3$ и элементарный интеграл

$$\int_0^\infty \frac{\sin r}{r} dr = \frac{\pi}{2}$$

легко показать, что для любого $\psi \in \mathscr{S}(\mathbb{R}^3)$

$$\frac{1}{2\pi^2\hbar} \int_{\mathbb{R}^3} \frac{\hat{\psi}(\boldsymbol{q})}{|\boldsymbol{p}-\boldsymbol{q}|^2} d^3\boldsymbol{q} = \frac{1}{(\sqrt{2\pi\hbar})^3} \int_{\mathbb{R}^3} \frac{1}{r} \psi(\boldsymbol{x}) e^{-\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{x}} d^3\boldsymbol{x}$$

где $\hat{\psi} = \mathscr{F}_\hbar(\psi)$ - зависящее от $\hbar$ преобразование Фурье [9].

Пусть ψ - собственная функция H с собственным значением $E < 0$. Из (5.24) следует, что в импульсном представлении соответствующее уравнение Шрёдингера - уравнение на собственные значения $H\psi = E\psi$ - принимает вид

$$\left(\boldsymbol{p}^2 + p_0^2\right) \hat{\psi}(\boldsymbol{p}) = \lambda \int_{\mathbb{R}^3} \frac{\hat{\psi}(\boldsymbol{q})}{|\boldsymbol{p}-\boldsymbol{q}|^2} d^3\boldsymbol{q}$$

где $p_0 = \sqrt{-2\mu E}$ и $\lambda = \frac{\alpha\mu}{p_0\hbar}$. Дальше рассмотрим однородные координаты $\frac{p}{p_0}$ в $\mathbb{R}^3$ как координаты стереографической проекции единичной сферы S^3 в $\mathbb{R}^4$. А именно: обозначив как n единичный вектор из начала координат в северный полюс S^3, получим для точки $u \in S^3$, соответствующей $\frac{\boldsymbol{p}}{p_0} \in \mathbb{R}^3$

$$u = \frac{p^2 - p_0^2}{p^2 + p_0^2}\boldsymbol{n} + \frac{2p_0}{p^2 + p_0^2}\boldsymbol{p}$$

[9] Поскольку $\boldsymbol{x}$ - переменная в координатном представлении, здесь $\boldsymbol{q}$ - другая переменная в импульсном представлении. Для формы объема на S^3 имеем

$$d\Omega = \frac{(2p_0)^3}{\left(\boldsymbol{p}^2 + p_0^2\right)^3} d^3\boldsymbol{p}, \quad \int_{S^3} d\Omega = 2\pi^2$$

Используя равенство

$$|\boldsymbol{p}-\boldsymbol{q}|^2 = \frac{\left(\boldsymbol{p}^2 + p_0^2\right)\left(\boldsymbol{q}^2 + p_0^2\right)}{(2p_0)^2} |\boldsymbol{u}-\boldsymbol{v}|^2,$$

где $\boldsymbol{v} \in S^3$ соответствует $\frac{\boldsymbol{q}}{p_0} \in \mathbb{R}^3$, и вводя

$$\Psi(\boldsymbol{u}) = \frac{1}{\sqrt{p_0}} \frac{\left(\boldsymbol{p}^2 + p_0^2\right)^2}{(2p_0)^2} \hat{\psi}(\boldsymbol{p}),$$

можно переписать уравнение (5.25) как

$$\Psi(\boldsymbol{u}) = \frac{\lambda}{2\pi^2} \int_{S^3} \frac{\Psi(\boldsymbol{v})}{|\boldsymbol{u}-\boldsymbol{v}|^2} d\Omega_{\boldsymbol{v}}$$

Имеем также

$$\int_{S^3} |\Psi(\boldsymbol{u})|^2 d\Omega_{\boldsymbol{u}} = \int_{\mathbb{R}^3} \frac{\boldsymbol{p}^2 + p_0^2}{2p_0^2} |\hat{\psi}(\boldsymbol{p})|^2 d^3\boldsymbol{p} = \int_{\mathbb{R}^3} |\hat{\psi}(\boldsymbol{p})|^2 d^3\boldsymbol{p}.$$

Действительно, из уравнения Шрёдингера следует, что

$$\frac{1}{2\mu}\int\limits_{\mathbb{R}^3}\boldsymbol{p}^2|\hat{\psi}(\boldsymbol{p})|^2d^3\boldsymbol{p}=\frac{1}{2\mu}\int\limits_{\mathbb{R}^3}\left|\frac{\partial\psi(\boldsymbol{x})}{\partial\boldsymbol{x}}\right|^2d^3\boldsymbol{x}=\int\limits_{\mathbb{R}^3}(E-V(r))|\psi(\boldsymbol{x})|^2d^3\boldsymbol{x},$$

и по теореме о вириале (см. раздел 3.1.3) получаем

$$\frac{1}{2\mu}\int\limits_{\mathbb{R}^3}\left|\frac{\partial\psi(\boldsymbol{x})}{\partial\boldsymbol{x}}\right|^2d^3\boldsymbol{x}=-\frac{1}{2\mu}\int\limits_{\mathbb{R}^3}\Delta\psi(\boldsymbol{x})\overline{\psi(\boldsymbol{x})}d^3\boldsymbol{x}=-\frac{1}{2}\int\limits_{\mathbb{R}^3}V(r)|\psi(\boldsymbol{x})|^2d^3\boldsymbol{x},$$

где $V(r)=-\frac{\alpha}{r}$, так что

$$\int\limits_{\mathbb{R}^3}V(r)|\psi(\boldsymbol{x})|^2d^3\boldsymbol{x}=2E\int\limits_{\mathbb{R}^3}|\psi(\boldsymbol{x})|^2d^3\boldsymbol{x}=2E\int\limits_{\mathbb{R}^3}|\hat{\psi}(\boldsymbol{p})|^2d^3\boldsymbol{p}.$$

Это показывает, что задача о собственных значениях уравнения Шрёдингера эквивалентна задаче о собственных значениях интегрального уравнения (5.26) на $L^2\left(S^3,d\Omega\right)$. Последняя - классическая задача теории сферических гармоник. А именно: функция $G(u)=-\frac{1}{4\pi^2u^2}$, где $u=|\boldsymbol{u}|$, $u\in\mathbb{R}^4$, - фундаментальное решение оператора Лапласа Δ на $\mathbb{R}^4$:

$$\Delta=\frac{\partial^2}{\partial u_1^2}+\frac{\partial^2}{\partial u_2^2}+\frac{\partial^2}{\partial u_3^2}+\frac{\partial^2}{\partial u_4^2}$$

а уравнение (5.26) - уравнение, которому удовлетворяют сферические гармоники на S^3: собственные функции сферической части Δ_0 оператора Лапласа на $\mathbb{R}^4$, определенного формулой

$$\Delta=\frac{1}{u^3}\frac{\partial}{\partial u}\left(u^3\frac{\partial}{\partial u}\right)+\frac{1}{u^2}\Delta_0$$

Хорошо известно из теории представлений группы Ли $SO(4)$, что сферические гармоники - это ограничения на S^3 однородных гармонических многочленов на $\mathbb{R}^4$ степени $n-1,n\in\mathbb{N}$. Соответственно, уравнение (5.26) получается как предел $|u|\to1$ формулы Грина для однородных гармонических функций степени $n-1$ в единичном шаре в $\mathbb{R}^4$ с использованием потенциала двойного слоя. Это дает $\lambda=n$, чем опять устанавливается точная формула для уровней энергии атома водорода. Изоморфизм $\mathscr{H}_0\simeq L^2\left(S^3,d\Omega\right)$ следует из (5.27), а (5.23) - из разложения

$$L^2\left(S^3,d\Omega\right)\simeq\bigoplus_{l\in\frac{1}{2}\mathbb{Z}_{\geqslant0}}V_l\otimes V_l$$

регулярного представления SO(4) в прямую сумму неприводимых компонент. Можно также получить явный вид (5.4) собственных функций, воспользовавшись теорией представлений SO(4). Мы оставляем все эти детали заинтересованному читателю.

ЗАМЕЧАНИЕ. При $E>0$ надо рассмотреть подпространство $\mathscr{H}_1=\mathrm{P}_H(0,\infty)\mathscr{H}$ и определить $\boldsymbol{J}^{(\pm)}=\frac{1}{2}\left(\boldsymbol{M}\pm(2H)^{-1/2}\boldsymbol{W}\right)$. Вместо (5.21) эти операторы удовлетворяют коммутационным соотношениям алгебры Ли $\mathfrak{so}(3,1)$ группы Лоренца SO(3,1). Задачу нахождения собственных функций непрерывного спектра для кулоновской задачи можно решить, используя гармонический анализ на трехмерном пространстве Лобачевского. ЗАДАЧА 5.1. Покажите, что компоненты углового момента $\boldsymbol{M}$ - образующие $\mathfrak{so}(4)$, соответствующие бесконечно малым вращениям в подпространстве $\mathbb{R}^4$ с координатами $(0,\boldsymbol{p})$, а компоненты вектора ЛапласаРунге-Ленца $\boldsymbol{W}$ соответствуют бесконечно малым вращениям в плоскостях (p_0p_1), (p_0p_2) и (p_0p_3) в $\mathbb{R}^4$.

6.5.5 Particle in a Central-Symmetric Potential by Takhtajan

Задача на собственные значения для оператора Шрёдингера

$$H = -\frac{\hbar^2}{2\mu}\Delta + V(\boldsymbol{x})$$

упрощается, когда H коммутирует с действием SO(3) на $\mathscr{H} = L^2\left(\mathbb{R}^3, d^3\boldsymbol{x}\right)$:

$$[H, T(g)] = 0 \quad \text{для любого } g \in \mathrm{SO}(3).$$

Это сводится к условиям

$$[H, M_i] = 0, \quad i = 1, 2, 3,$$

и эквивалентно свойству, что потенциал V сферически симметричен, $V(\boldsymbol{x}) = V(r), r = |\boldsymbol{x}|$. В частности,

$$[H, M_3] = \left[H, M^2\right] = 0$$

где $M^2 = M_1^2 + M_2^2 + M_3^2$, а операторы M_3 и M^2 - коммутирующие интегралы движения для гамильтониана H. Как следует из результатов раздела 3.3.2, можно искать решения задачи на собственные значения

$$H\psi = E\psi$$

удовлетворяющие условию

$$M_3\psi = m\psi \quad \text{и} \quad M^2\psi = \hbar^2 l(l+1)\psi, \quad m = -l, ..., l$$

Используя (3.9), получаем

$$H = -\frac{\hbar^2}{2\mu r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{M^2}{\mu r^2} + V(r)$$

так что в согласии с разложениями (3.14) и (3.15) мы ищем решения в виде

$$\psi(\boldsymbol{x}) = R_l(r)Y_{lm}(\boldsymbol{n}), \quad \boldsymbol{x} = r\boldsymbol{n}$$

где Y_{lm} - нормированные сферические функции. Разделяя переменные, получаем следующее обыкновенное дифференциальное уравнение на функцию $R_l(r)$:

$$\frac{\hbar^2}{2\mu r^2}\frac{d}{dr}\left(r^2\frac{dR_l}{dr}\right) + \frac{\hbar^2 l(l+1)}{\mu r^2}R_l + V(r)R_l = ER_l$$

ВвОдЯ

$$f_l(r) = rR_l(r)$$

получаем так называемое радиальное уравнение Шрёдингера:

$$-\frac{\hbar^2}{2\mu}\frac{d^2 f_l}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2}f_l + V(r)f_l = Ef_l.$$

Поскольку для непрерывного потенциала $V(\boldsymbol{x})$ решение $\psi(\boldsymbol{x})$ также непрерывно, уравнение (4.10) следует дополнить граничным условием $f_l(0) = 0$. Радиальное уравнение Шрёдингера выглядит аналогичным уравнению Шрёдингера для одномерной частицы, если ввести так называемый эффективный потенциал

$$V_{\text{eff}}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2}$$

в котором второе слагаемое называется центробежной энергией. Однако, поскольку f_l определено только при $r > 0$, уравнение (4.10) эквивалентно уравнению (2.1) с потенциалом, удовлетворяющим условию $V(x) = \infty$ при $x < 0$, описывающим бесконечный потенциальный барьер при $x = 0$.

Поскольку радиальные операторы Шрёдингера

$$H_l = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2}$$

получаются из трехмерного оператора Шрёдингера

$$H = -\frac{\hbar^2}{2\mu}\Delta + V(r)$$

разделением переменных, операторы H_l самосопряжены в $L^2(0,\infty)$, если H - самосопряженный оператор в $L^2(\mathbb{R}^3)$. Оператор H_0 следует дополнить граничным условием $f_0(0) = 0$, тогда как в случае $l > 0$ никаких граничных условий не требуется. В частности, из теоремы 1.9 в разделе 3.1.2 следует, что если ограниченный потенциал V удовлетворяет условию

$$V(r) = O\left(r^{-1-\varepsilon}\right) \quad \text{при} \quad r \to \infty$$

для некоторого $\varepsilon > 0$, то H_l - самосопряженные операторы с простым абсолютно непрерывным спектром, заполняющим $[0,\infty)$, и отрицательными собственными значениями с возможной точкой сгущения в нуле. Если

$$V(r) = O\left(r^{-2-\varepsilon}\right) \quad \text{при} \quad r \to \infty$$

то у операторов H_l конечно число отрицательных собственных значений, а при достаточно больших l собственных значений вообще нет. Такое же заключение верно, если

$$\int_0^\infty r|V(r)|dr < \infty$$

Такие потенциалы $V(r)$ называются короткодействующими потенциалами. Затухающие на бесконечности потенциалы, не удовлетворяющие (4.11), называются дальнодействуючими потенциалами. Для короткодействующего потенциала $V(r)$ дифференциальное уравнение (4.10) при $E \neq 0$ имеет два линейно независимых решения $f_l^{\pm}(r)$, удовлетворяющих следующим асимптотикам при $r \to \infty$:

$$f_l^{\pm}(r) = e^{\pm \varkappa r}(1 + o(1)),$$

где $\varkappa = \sqrt{-2\mu E}$ чисто мнимое, $\operatorname{Im}\varkappa > 0$ при $E > 0$ и $\varkappa > 0$ при $E < 0$. Когда $r \to 0$, наиболее сингулярный член в радиальном уравнении Шрёдингера дается центробежной энергией. Поскольку элементарное дифференциальное уравнение

$$f'' = \frac{l(l+1)}{r^2} f$$

имеет два линейно независимых решения r^{-l} и r^{l+1}, решение $f_l(r)$, удовлетворяющее граничному условию $f_l(0) = 0$, имеет асимптотику

$$f_l(r) = Cr^{l+1} + o(1) \quad \text{при} \quad r \to 0$$

и однозначно определено (с точностью до константы). Поскольку

$$f_l(r) = C_1 f_l^+(r) + C_2 f_l^-(r)$$

для некоторых констант C_1 и C_2, зависящих от E, у дифференциального уравнения (4.10) нет решений с интегрируемым квадратом при $E > 0$. Соответствующее решение $f_l(r)$ ограничено на $[0, \infty)$ и является собственной функцией непрерывного спектра. Это согласуется с описанием в разделе 1.1.6 главы 1, поскольку при $E > 0$ классическая частица в центральном потенциале $V_{\text{eff}}(r)$ уходит на бесконечность с конечной скоростью. При $E < 0$ уравнение $C_1(E) = 0$ определяет собственные значения H_l, которые просты. Это тоже согласуется с классической картиной, поскольку классическое движение финитно при $E < 0$. Для короткодействующего потенциала уравнение $C_1(E) = 0$ имеет лишь конечное число решений. Когда $V_{\text{eff}}(r) > 0$ при $r > 0$ - случай отталкивающего потенциала, у оператора H_l нет собственных значений.

ЗАмЕчАНиЕ. Когда $V(r) = 0$, радиальный оператор Шрёдингера H_l имеет только простой абсолютно непрерывный спектр, заполняющий $[0, \infty)$. Подстановка

$$f_l(r) = \sqrt{\xi} J(\xi), \quad \xi = \frac{kr}{\hbar} \quad \text{и} \quad k = |\varkappa| = \sqrt{2\mu E} > 0$$

сводит дифференциальное уравнение (4.10) к уравнению Бесселя

$$\xi^2 \frac{d^2 J}{d\xi^2} + \xi \frac{dJ}{d\xi} + \left(\xi^2 - \nu^2\right) J = 0$$

полуцелого порядка $\nu = l + \frac{1}{2}$. Соответствующее решение, регулярное в нуле, - функция Бесселя первого рода $J_{l+\frac{1}{2}}(\xi)$ - явно дается формулами

$$J_{l+\frac{1}{2}}(\xi) = (-1)^l \sqrt{\frac{2}{\pi\xi}} \xi^{l+1} \left(\frac{1}{\xi}\frac{d}{d\xi}\right)^l \frac{\sin\xi}{\xi}$$

и

$$J_{l+\frac{1}{2}}(\xi) = \sqrt{\frac{2}{\pi\xi}} \sin\left(\xi - \frac{l\pi}{2}\right) + O\left(\xi^{-1}\right) \quad \text{при} \quad \xi \to \infty$$

Можно показать, что

$$f_{El}(r) = \sqrt{\frac{kr}{\hbar}} J_{l+\frac{1}{2}}\left(\frac{kr}{\hbar}\right)$$

удовлетворяют условию нормировки (2.14) из раздела 2.2.2 главы 2:

$$\lim_{\Delta\to 0} \frac{1}{\Delta} \int_0^\infty \left(\int_k^{k+\Delta} f_{El}(r) d\sigma(E) \right)^2 dr \equiv 1$$

где $k = \sqrt{2\mu E}$ и $d\sigma(E) = \sqrt{\frac{\mu}{2E}} dE = dk$. Соответствующая теорема о разложении по собственным функциям - особый случай классического преобразования Фурье-Бесселя для целого l, обобщающего синусоидальное преобразование Фурье: для любого $f \in L^2(0, \infty)$

$$f(r) = \int_0^\infty c_l(E) f_{El}(r) d\sigma(E), \quad c_l(E) = \int_0^\infty f(r) f_{El}(r) dr$$

В общем случае для любого $l = 0, 1, ...$, обозначим как $f_{El}(r)$ решение радиального уравнения Шрёдингера (4.10) со следующей асимптотикой:

$$f_{El}(r) = \sqrt{\frac{2}{\pi\hbar}} \sin\left(\frac{kr}{\hbar} - \frac{l\pi}{2} + \delta_l\right) + o(1) \quad \text{при} \quad r \to \infty$$

Функция $\delta_l(k), k = \sqrt{2\mu E}$, называется фазовым сдвигом. Из (4.14) следует, что для случая свободного движения $\delta_l(k) = 0$. Собственные функции непрерывного спектра $f_{El}(r)$ удовлетворяют тому же условию нормировки (4.15), что и собственные функции для случая свободного движения. Функция $S_l(k) = e^{2i\delta_l(k)}$ играет роль матрицы рассеяния для радиального оператора Шрёдингера H_l. Она допускает мероморфное продолжение в верхнюю полуплоскость $\operatorname{Im} k > 0$ с простыми полюсами $k = i\varkappa_{kl} = i\sqrt{-2\mu E_{kl}}$, где E_{kl} - собственные значения H_l.

Пусть $E_{0l} < E_{2l} < \cdots < E_{N_l-1l} < 0$ - собственные значения H_l, и пусть $f_{jl}(r), j = 0, ..., N_l - 1$, - соответствующие нормированные собственные функции. По теореме о колебаниях собственные функции $f_{jl}(r)$ имеют j простых нулей на $(0, \infty)$. Функции

$$\psi_{jlm}(\boldsymbol{x}) = \frac{f_{jl}(r)}{r} Y_{lm}(\boldsymbol{n}), \quad m = -l, ..., l$$

это нормированные собственные функции оператора Шрёдингера H с собственными значениями E_{jl}, а функции

$$\psi_{Elm}(\boldsymbol{x}) = \frac{f_{El}(r)}{r} Y_{lm}(\boldsymbol{n}), \quad m = -l, ..., l$$

это нормированные собственные функции непрерывного спектра. Соответствующая теорема о разложении по собственным функциям для оператора Шрёдингера H со сферически симметричным потенциалом утверждает, что для любого $\psi \in L^2(\mathbb{R}^3, d^3\boldsymbol{x})$

$$\psi(\boldsymbol{x}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \int_0^{\infty} c_{lm}(E)\psi_{Elm}(\boldsymbol{x}) d\sigma(E) + \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{j=0}^{N_l-1} c_{jlm}\psi_{jlm}(\boldsymbol{x})$$

где

$$c_{lm}(E) = \int_{\mathbb{R}^3} \psi(\boldsymbol{x})\overline{\psi_{Elm}(\boldsymbol{x})} d^3\boldsymbol{x}, \quad c_{jlm} = \int_{\mathbb{R}^3} \psi(\boldsymbol{x})\overline{\psi_{jlm}(\boldsymbol{x})} d^3\boldsymbol{x}.$$

ЗАМЕЧАНИЕ. В физике параметр j собственной функции $\psi_{jlm}(\boldsymbol{x})$ традиционно называется радиальным квантовым числом и обозначается n_r. Параметр l называется азимутальным квантовым числом, а параметр m - магнитным квантовым числом. Эта терминология происходит из старой квантовой теории, в которой каждому значению E_{kl} соответствует классическая орбита. Параметр $n = n_r + l + 1$ называется главным квантовым числом, так что $n_r = n - l - 1$ - всегда количество нулей соответствующей радиальной собственной функции $f_{jl}(r)$.

ЗАМЕЧАНИЕ. В общем случае собственные значения E_{jl} оператора Шрёдингера H со сферически симметричным потенциалом имеют кратность $2l + 1$. Для особых потенциалов, благодаря дополнительным симметриям задачи, могут возникать «случайные вырождения» относительно азимутального квантового числа l. Таков случай оператор Шрёдингера атома водорода, который мы будем рассматривать в следующем разделе.

ЗАдАЧА 4.7. Докажите все результаты, приведенные в этом разделе. (Указание: см. литературу к этой главе.)

ЗАдАЧА 4.8. Найдите уровни энергии частицы с угловым моментом $l = 0$ в центрально-симметричной потенциальной яме $V(r) = -V_0 < 0$ при $0 < r < a$ и $V(r) = 0$ при $r > a$.

ЗАдАЧА 4.9. Найдите спектр оператора Шрёдингера с потенциалом $V(r) = ar^{-2} + br^2, a, b > 0$.

ЗАДАЧА 4.10. Докажите, что рассеянная волна $u(\boldsymbol{x}, \boldsymbol{k}) = u^{(+)}(\boldsymbol{x}, \boldsymbol{k})$ в центрально-симметричном потенциале дается формулой

$$u(\boldsymbol{x}, \boldsymbol{k}) = \frac{1}{kr}\sqrt{\frac{\pi}{2}}\sum_{l=0}^{\infty}(2l+1)i^l e^{i\delta_l(k)} f_{El}(r)P_l(\cos\vartheta)$$

где $\boldsymbol{x}\cdot\boldsymbol{k} = kr\cos\vartheta$ и, как в разделе 3.4.2, $\hbar = 1$, а $\mu = \frac{1}{2}$.

ЗАдАЧА 4.11. Используя результат предыдущей задачи, покажите, что

$$f(k, \boldsymbol{n}, \boldsymbol{\omega}) = f(k, \cos\vartheta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left(S_l(k) - 1\right)P_l(\cos\vartheta)$$

разложение амплитуды рассеяния по парчиальным волнам, и получите следующую формулу для полного сечения:

$$\sigma_{\text{tot}}\,(k) = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l(k)$$

6.5.6 Other Questions About the Central Field

Падение частицы на центр по Ландау

(ну да, тут отдельно это можно исследовать, а мне так лень...)

Для выяснения некоторых особенностей квантовомеханического движения полезно изучить случай, не имеющий, правда, непосредственного физического смысла,- движение частицы в поле с потенциальной энергией, обращающейся в некоторой точке (начале координат) в бесконечность по закону $U(r) \approx -\beta/r^2(\beta > 0)$; вид поля вдали от начала координат нас не будет интересовать. Мы видели в §18, что этот случай - как раз промежуточный между теми, когда имеются обычные стационарные §35 ПАДЕНИЕ ЧАСТИЦЫ НА ЦЕНТР 151 состояния, и случаями, когда происходит «падение» частицы в начало координат.

Вблизи начала координат уравнение Шредингера в рассматриваемом случае будет следующим:

$$R'' + \frac{2}{r}R' + \frac{\gamma}{r^2}R = 0$$

($R(r)$ - радиальная часть волновой функции), где введена постоянная

$$\gamma = \frac{2m\beta}{\hbar^2} - l(l+1)$$

и опущены все члены более низкого порядка по $1/r$; значение энергии E предполагается конечным, и потому соответствующий член в уравнении тоже опущен.

Ищем R в виде $R \sim r^s$; тогда получаем для s квадратное уравнение

Так в итоге, если частица падает на центр, то она там и останется что ли? (????)

(пока хз.)

6.5.7 Central Field in Spherical and Parabolic Coordinates

(лл3, там приводится это.)

Движение в кулоновском поле (сферические координаты) по Ландау

Движение в кулоновском поле (параболические координаты) по Ландау

Особенности квантового движения

В отличие от классической механики движение не плоское (????)

(потом подробнее про это напишу)

6.5.8 Non-Relativistic Hydrogen Atom

Обсудим подробно нерелятивистский атом водорода.
(очень скоро напишу нормально!)

Атом водорода в двух словах

(тут вся самая суть с формулами)

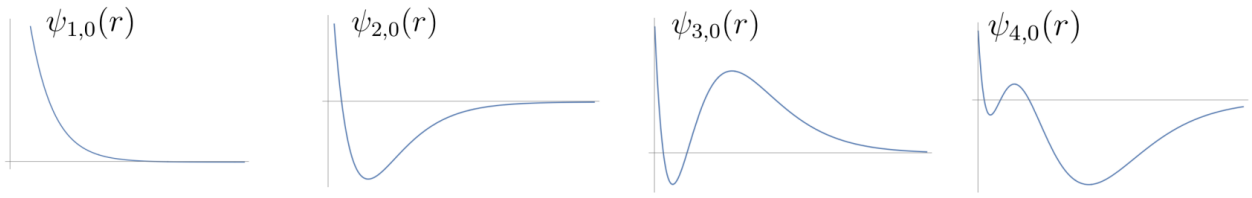


Figure 6.3: The (un-normalised) s-wave states for n = 1, 2, 3 and 4. The functions are plotted on the same range along the x-axis, although the y-axis range varies. Although it's not obvious from these plots, all wavefunctions approach a finite value at x = 0.

Модель нерелятивистского атома водорода

(тут подробно)
Кулоновский потенциал притяжения электрона и протона в атоме водорода в пренебрежении (?) имеет вид

$$V(r) = -\frac{e^2}{r}$$

Поэтому стационарное уравнение Шредингера имеет решения, которые разлагаются по ба
(???).
$\hat{H}$ -энергия стационарного уравнения Шредингера для радиального движения

$$-\frac{\hbar^2}{2m}u'' + \left\{-\frac{e^2}{r} + \frac{\hbar^2 l(l+1)}{2mr^2}\right\} u = Eu$$

так что радиальная волновая функция

$$R_l^E(r) = \frac{1}{r}u(r)$$

где $u(r) \sim r^{l+1}, \quad r \to 0,$

(???)

$$m = \frac{m_e m_p}{m_e + m_p}$$

(??)

сферическими гармониками

$$\hat{\boldsymbol{l}}^2 Y_{l,m}(\theta, \phi) = l(l+1) Y_{l,m}(\theta, \phi)$$

и

$$\hat{\boldsymbol{l}}_z Y_{l,m}(\theta, \phi) = m Y_{l,m}(\theta, \phi)$$

4.P - четность с собственным и Значен иям и

$$\lambda_P = (-1)^l$$

Для полного определения волновой функции стационарного состояния

$$\Psi_{l,m}(\boldsymbol{r}) = R_l^E(r) Y_{l,m}(\theta, \phi)$$

необходимо решить радиальное уравнение (11.2)

с эффективным потенциалом, учитывающим вклад орбитального движения, как показано на рис.

количественные выводы из модели атома водорода

??? сколько там всего уровней энергии? как решаем УШ для них?
это такие, которые состоят из двух частиц и связаны только электрическими силами.
это He^+, Li^+, Be^{+++}, я вообще хз, почему они сюда относятся, потом пойму.

качественный вид волновых функций атома водорода

Приведем визуальное представление волновых функций
(как же давно уже хочу дойти сюда!!!)

модель атома водорода в 2D

Определим уровни энергии, кратности их вырождения, стационарные волновые функции для двумерной частицы, движущейся в притягивающем потенциале $U(r) = \frac{e^2}{r}$.

Уравнение Шредингера для этой модели имеет вид

$$u''_{rr} + \frac{1}{r} u'_r + \frac{1}{r^2} u''_{\phi\phi} - 2M \left(-\frac{e^2}{r} + E \right) u = 0;$$

где $E > 0$.

ищем решение в виде $u(r, \phi) = \psi(r) e^{im\phi}$, где $m \in Z$,

$$r\psi''_{rr} + \psi'_r + \left(2Me^2 - 2MEr - \frac{m^2}{r} \right) \psi = 0$$

Если $\psi(r) = f(r) r^a$, то

$$r^{a+1} f'' + (2a+1) r^a f' + \left(a^2 r^{a-1} - m^2 r^{a-1} + 2Me^2 r^a - 2MEr^{a+1} \right) f = 0$$

положим $a = m$, тогда

$$rf'' + (2m+1)f' + \left(2Me^2 - 2MEr\right) f = 0$$

и также $f(r) = F(r)e^{br}$, получаем

$$rF'' + (2br + (2m+1))F' + \left(b^2 r + (2m+1)b + 2Me^2 - 2MEr\right) F = 0$$

видим, что польза есть от $b = -\sqrt{2ME}$, получаем

$$rF'' + (-2\sqrt{2ME}r + (2m+1))F' + \left(-(2m+1)\sqrt{2ME} + 2Me^2\right) F = 0$$

$$F(r) =_1 F_1\left(-\frac{\left(-(2m+1)\sqrt{2ME} + 2Me^2\right)}{2\sqrt{2ME}}, 2m+1, 2\sqrt{2ME}r\right)$$

В итоге

$$\psi(r) = r^m e_1^{-\sqrt{2ME}r} F_1\left(-\frac{\left(-(2m+1)\sqrt{2ME} + 2Me^2\right)}{2\sqrt{2ME}}, 2m+1, 2\sqrt{2ME}r\right)$$

для конечности волновой функции необходимо, чтобы $\frac{\left(-(2m+1)\sqrt{2ME}+2Me^2\right)}{2\sqrt{2ME}} = n$ в итоге m кратно вырожденные уровни:

$$E = \frac{M}{2}\frac{e^4}{\left(n + \left(m + \frac{1}{2}\right)\right)^2}$$

Обзор применений методов описания атома водорода в других задачах и науках (??)

(укажу, где будет она нужна)

6.6 Three-Dimensional Problem by Migdal-Krainov (?)

6.6.1 Centrally-Symmetric Field

Рассмотрим квазиклассическое движенне в центральносимметричном поле. Переменные $0, \varphi$ в этом случае отделяются от перємной r:

$$\Psi_{nlm} = R_{nl}(r)Y_{lm}(\theta, \varphi).$$

Расснотрим сначала радиäльную часть волновой функции. Введем функцно

$$u_{nl}(r) = rR_{nl}(r).$$

From ограниченности $R_{ni}(r)$ при $r = 0$ следует, что $u_{ni}(0) = 0$. Дла u_{nl}, как нзвестно, получается одномерное уравнение

$$u''_{nl} + k^2_{nl} u_{nl} = 0$$

где

$$k^2_{nl} = 2\left[\varepsilon_{nl} - V(r) - \frac{l(l+1)}{2r^2}\right].$$

Условие $u_{n2}(0) = 0$ соответствует в одномерной задаче бесконечной потенциальной стенке в начале координат.

Прн увеличении l и заданном $V(r)$ яма на рис. 28 сталовится все мельче и в конце концов исчезает, т. е. при достаточио большом l система не будет обладать дйсретныни уровнпми. Значениям $\varepsilon_{nl} > 0$ соответствует сплоціной спектю.

6.6.2 Energy Levels in a Coulomb Field

Найдем уровни энергии в кулоновском поле. Условие квантования имеет вид (при $l \neq 0$, рнс. 28,б)

$$\int_{r_{\min}}^{\max_{\max}} \sqrt{2\left(E_n + \frac{Z}{r} - \frac{(l+1/2)^2}{2r^2}\right)} dr = \left(n_r + \frac{1}{2}\right)\pi.$$

Здесь n_r - радиальное квантовое число, $r_{\min}, r_{\max}$ - квазиклассические точки поворота. Мы заменили в центробежном потенциале $l(l+1) \to (l+1/2)^2$. Тогда квазиклассическая функция имеет фазу на бесконечности, совпадающую с точным решением, между тем как другие величины от такой замены практически не меняются. Интеграл в левой части приведенного выше условия равен

Следовательно,

$$\frac{Z\pi}{\sqrt{-2E_n}} - \left(l + \frac{1}{2}\right)\pi.$$

$$E_n = -\frac{Z^2}{2n^2},$$

где $n = n_r + l + 1$ - главное квантовое число.

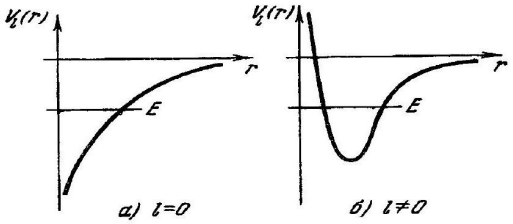


Рис. 28.

При $l = 0$ (рис. $28, a$) левая точка поворота $r_{\min} = 0$ и совпадает с особой точкой уравнения, т. е. в области левой точки поворота потенциал нельзя заменить прямой линией, как мы делали выше. Поэтому условие сшивки на левом краю изменится.

Для нахождения энергетических уровней при $l = 0$ нужно найти точное решение вблизи особой точки и сшить его с квазиклассическим решением вдали от нее.

Для больших квантовых чисел (т. е. энергий, близких к нулю), волновая функция в кулоновском поле с $l = 0$ имеет вид *)

$$R_{n0} = a_1 Z^{3/2} \frac{J_1\left(\sqrt{8Z_r}\right)}{\sqrt{Zr}},$$

где a_1 - нормировочный коэффициент. При $r \geqslant 1/Z$ отсюда находим

$$R_{n0} = a_1 \frac{\cos(\sqrt{8Zr} - 3/4\pi)}{r^{3/4}}.$$

С другой стороны, для R_{n0} можно написать квазиклассическое решение

$$R_{n0} = a_2 \frac{\cos\left(\int\limits_0^r p_r dr - C_1\pi\right)}{r\sqrt{p_r}} = a_2 \frac{\cos\left(\sqrt{8Zr} - C_1\pi\right)}{r\sqrt{p_r}}.$$

Таким образом, здесь появляется фаза $C_1\pi = \frac{3}{4}\pi$ вместо $\frac{1}{4}\pi$ в обычном случае. Функция R_{n0} может быть также записана в виде

$$R_{n0} = a_3 \frac{\cos\left(\int\limits_r^{r^{\max}} p_r dr - \pi/4\right)}{r\sqrt{p_r}}.$$

Здесь $r_{\max}$ - правая точка новорота. Из условия однозначности, так же как и в 3.1, получаем правило квантования

$$\int\limits_0^{r_{\max}} p_r dr = (n_r + 1)\,\pi = n\pi,$$

где n-главное квантовое число.

Вычисление интеграла даст

$$E_n = -\frac{Z^2}{2n^2}.$$

Как мы видим, в этом случае квазиклассическое приближение (так же как и в случае осциллятора) дает точные уровни энергий.

6.6.3 Quasi-Classical Representation of Spherical Functions

Для вычисления матричных элементов физических величин при больших угловых моментах l удобно использовать квазиклассическое представление для сферической функции:

$$Y_{lm}(\theta, \varphi) = \frac{1}{\sqrt{2\pi}} P_{lm}(\cos\theta) e^{imp}.$$

Здесь $P_{lm}(x)$ - присоединенный полином Jeeандра, удовлетворяющий уравнению

$$\frac{d}{dx}\left[\left(1 - x^2\right)\frac{dP_{L_m}}{dx}\right] + \left[l(I+1) - \frac{m^2}{1-x^2}\right] P_{tm} = 0.$$

Введем функцию $\vartheta_{lm}(x)$:

$$P_{lm}(x) = \frac{1}{\sqrt{1-x^2}} \vartheta_{lm}(x).$$

Тогда для $\vartheta_{tm}(x)$ имеем

$$\left(1 - x^2\right)\vartheta''_{lm}(x) + \left[l(l+1) - \frac{m^2+1}{1-x^2}\right]\vartheta_{lm}(x) = 0.$$

Решение этого уравнения с точностью порядка $1/l^2$ может быть найдено в квазиклассическом виде

$$\theta_{lm}(x) = \frac{a}{\sqrt{k}} \cos\left(\int\limits_{x_1}^{x} k dx - \frac{\pi}{4}\right),$$

где

$$k^2(x) = \frac{1}{1-x^2}\left[\left(l+\frac{1}{2}\right)^2 - \frac{m^2}{1-x^2}\right].$$

В точках $x_{1,2}$ величина $k(x)$ обращается в нуль, т.е.

$$x_{1,2} = \mp\sqrt{1-\frac{m^2}{(l+1/2)^2}}.$$

Мы заменили здесь $l(l+1) \longrightarrow (l+1/3)^2$, имея в виду, что квазиклассическое приближение применияо с точностью до $1/t^2$ (а не $1/l$; см. 3.1).

Коэффициент a определяется из условня нормировки присоединенных полиномов Лежандра:

$$int_{-1}^{1} P_{lm}^2(x)dx = 1,$$

т.е.

Вычислим

$$\int_{x_1}^{x_2^2}\int_{x_1}^{x_2}\frac{1}{1-x^2}\frac{dx}{k} = 1 = \frac{a^2}{2}\frac{1}{l+\frac{1}{2}}\frac{\partial}{\partial l}\int_{x_1}^{x_2} kdx.$$

$$\int_{x_1}^{x_2}\sqrt{\frac{1}{(1-x^2)}\left[\left(l+\frac{1}{2}\right)^2 - \frac{m^2}{1-x^2}\right]}dx = \left(l-|m|+\frac{1}{2}\right)\pi.$$

Этот результат следовало ожидать, так ікак число узлов $P_{tm}(x)$, как известно, равно $l-|m|$. Из (3.25) находим

$$\frac{\partial}{\partial l}\int_{x_1}^{x_2} kdx = \pi$$

Следовательно,

$$a^2 = \frac{2l+1}{\pi}.$$

Окончательно имеем

$$P_{lm}(x) \underset{x_1<x<x_2}{=} \sqrt{\frac{2l-1}{\pi}}\frac{1}{\sqrt{1-x^2}}\frac{1}{\sqrt{k}}\cos\left(\int_{x_1}^{x} kdx - \frac{\pi}{4}\right),$$

где

$$k = \frac{1}{\sqrt{1-x^2}}\pi\sqrt{\left(l+\frac{1}{2}\right)^2 - \frac{m^2}{1-x^2}}$$

Квазиклассическое представление сферических функций позволяет приближенно вычислять суммы вида

$$I_l(\theta) = \sum_{m=-t}^{l} |Y_{lm}(\theta,\varphi)|^2\,\Phi(m).$$

Действительно, используя условие квантования (3.25) и заменяя суммирование интегрированием, получаем

$$I_l(\theta) = \frac{l+1/2}{2\pi^2} \int\limits_{-(l+1/2)|\sin\theta|}^{(l+1/2)|\sin\theta|} \frac{\Phi(m)dm}{(l+2)\sin\theta\sqrt{1-\frac{m^2}{(l+1/2)^2\sin^2\theta}}} =$$

$$= \frac{l+1/2}{2\pi^2} \int\limits_{-1}^{1} \frac{dt}{\sqrt{1-t^2}} \Phi[t(l+1/2)\sin\theta].$$

В частности, для $\Phi(m) = 1, m^2, m^4$ находим

$$\sum_{m=-l}^{l} |Y_{lm}|^2 = \frac{l+1/2}{2\pi^2} \int\limits_{-1}^{1} \frac{dt}{\sqrt{1-t^2}} = \frac{2l+1}{4\pi},$$

$$\sum_{m=-l}^{l} |Y_{lm}|^2 m^2 = \frac{l+1/2}{2\pi^2} \int\limits_{-1}^{1} \frac{dt}{\sqrt{1-t^2}} t^2 (l+1/2)^2 \sin^2\theta = \frac{(l+1/2)^3}{4\pi} \sin^2\theta.$$

$$\sum_{m=-l}^{l} |Y_{lm}|^2 m^4 = \frac{l+1/2}{2\pi^2} \int\limits_{-1}^{1} \frac{dt}{\sqrt{1-t^2}} t^4 (l+1/2)^4 \sin^4\theta = \frac{3(l+1/2)^5}{16\pi} \sin^4\theta.$$

6.6.4 Thomas-Fermi Distribution in the Atom

Для потенциала V атома можно написать следующее электростатическое уравнение:

$$\Delta V = -4\pi\rho,$$

где ρ - плотность заряда электронов в данной точке. Это уравнение приближенное, так как на самом деле мы имеем многочастичную задачу - ядро и Z электронов - и потенциал

$$V(\boldsymbol{r}, \boldsymbol{r}_i) = -\frac{Z}{r} + \sum_{i=1}^{Z} \frac{1}{|\boldsymbol{r} - \boldsymbol{r}_i|}$$

есть оператор, а не число, т. е. V зависит от электронных координат, в то время как ρ, очевидно, нет. Следовательно, потенциал, используемый в (3.26), есть значение истинного потенциала, усредненное по движению электронов.

Поскольку частиц много, то отклонения $V(\boldsymbol{r}, \boldsymbol{r}_i)$ от $V(\boldsymbol{r})$ будут в среднем малы (хотя формально $V(\boldsymbol{r}, \boldsymbol{r}_i)$ может принимать любые значения). У равнение Шредингера с таким усредненным потенциалом имеет вид

$$\Delta\Psi + 2(E - V)\Psi = 0,$$

причем потенциал V можно сiитать сферически-симметричным (сферическая симметрия может нарушаться лишь за счет наружных электронов или незаполненных оболочек). Тогда $\Psi_{nlm} = \frac{u_{nl}(r)}{r} Y_{lm}$, причем для $u_{nl}(r)$ имеем уравнение

$$u''_{nl} + k^2_{nl} u_{nl} = 0,$$

где

$$k^2_{nl} = 2\left[E - V(r) - \frac{l(l+1)}{2r^2}\right].$$

Функция u_{nl} удовлетворяет граничным условиям

$$u_{nl}(0) = 0, \quad \lim_{r\to\infty} u_{nl}(r) = 0$$

и нормирована следующим образом:

$$\int_0^\infty u_{nl}^2 dr = 1.$$

(функцию $u_{n\mathrm{Im}ath}$ можно считать вещественной). Плотность заряда электронов равна (как и всюду, $e = \hbar = m = 1$)

$$\rho = -2\sum_{nlm} |\Psi_{nlm}|^2 = -2\sum_{nlm} \frac{u_{nl}^2}{r^2} |Y_{lmn}|^2 .$$

Суммирование по m с учетом соотношения (стр. 140)

$$\sum_{m=-l}^{t} |Y_{lm}|^2 = \frac{2l+1}{4\pi}$$

приводит к выражению

$$\rho(r) = -2\sum \frac{u_{nl}^3(r)}{r^2}\frac{2l+1}{4\pi}.$$

В квазиклассическом приближении радиальная волновая функция имеет вид

$$u_{nl}(r) = \frac{a_{nl}}{\sqrt{k_{nl}}} \cos\left(\int_{r_1}^{r} k_{nl}dr - \frac{\pi}{4}\right),$$

где

$$k_{nl}^2(r) = E_{nt} - V(r) - \frac{(l+1/2)^2}{2r^2}, a_{nl}^2 \approx \frac{2}{\pi}\frac{\partial E_{nl}}{\partial n}.$$

Уровни энергии E_{nt} находятся из иравила кваитовация Бора

$$\int_{r_2}^{r_3} k_{ni}dr = \left(n + \frac{1}{2}\right)\pi.$$

При $l = 0$ вместо $n + 1/2$ в соотношении (3.31) нужно написать n (см. стр. 137). Из (3.29) и (3.30) получаем

$$\rho(r) = -\frac{1}{2\pi}\sum_{nl} \frac{a_{nl}^2}{k_{nl}r^2}(2l+1)\cos^2\left(\int_{r_1}^{r} k_{nl}dr - \frac{\pi}{4}\right).$$

В квазиклассическом приближении можно заменить средпее значение квадрата косинуса на 1/2. Из (3.32) имеем

$$\rho(r) = -\frac{1}{2\pi^2}\sum_{nl} \frac{\partial E_n t}{\partial n}\frac{2l+1}{r^2}\frac{1}{k_{nl}}.$$

От суммирования по n в (3.33) перейдем к интегрированию при фиксированном l; так как

$$\sum_n \frac{\partial E_{nl}}{\partial n}(...) \to \int \frac{\partial E_{nl}}{\partial n} dn(...) \to \int dE(...),$$

ТО

$$\sum_n \frac{\partial E_{nl}}{\partial n}\frac{1}{k_{nl}} = \int \frac{dE}{k_{nl}} = \int \frac{dE}{\sqrt{2\left(E - V_l\right)}} = \sqrt{2\left(E - \bar{V}_l\right)}\Big|_{E_{\min}}^{0},$$

где $E_{\min} = V_l$ (при $E > V_l$ волновая функцня имеет вид $\cos\left(\int kdr - \frac{\pi}{4}\right)$, а при $E < V_t$ она затухает экспоненциально и вкладом этоff части в $\rho(r)$ можно иренебречь). Поэтому выражение (3.33) можно запнсать в виде

$$\rho(r) = -\frac{1}{2\pi^2}\sum_l \frac{2l+1}{r^2}\sqrt{-2V_l}.$$

Так как $V_l = V + \frac{1}{2r^2}\left(l + \frac{1}{2}\right)^2$, то $\frac{dV_l}{dl} = \frac{2l\cdot -1}{r^2}$, так что (3.34) принимает вид

$$\rho(r) = -\frac{1}{\pi^2}\sum_l \frac{dV_l}{dl}\sqrt{-2V_l} = -\frac{1}{\pi^2}\int \sqrt{-2V_l}c'V_l =$$

$$= -\frac{2}{3\cdot 2\pi^2}\left(-2V_t\right)^{3/2}\Big|_{V_{\min}}^{V_{l_{\max}}}.$$

$V_{l_{\min}}$ соответствует $l = 0, V_{l_{\min}} = V$. Величина $V_{l_{\max}}(r) = 0$. Для состояний с бОльшими l точка r находится в классически недоступной области, и такие состояния вносят экспоненциально малый вклад в плотность в точке r (рис. 29). Итак,

$$\rho(r) = \frac{1}{3\pi^2}(-2V)^{3/2}.$$

Обозначая $-V \equiv \varphi$, запишем уравнение Пуассона (3.26: с учетом (3.36) в следующем виде:

$$\Delta\varphi = 4\pi\rho = \frac{8\sqrt{2}}{3\pi}\varphi^{3/s} = C\varphi^{3/2},$$

где $C \equiv 8\sqrt{\bar{2}}/3\pi$. Это - так называемое уравнение Томаса-Ферми. Рис. 29. Если $r \longrightarrow 0$, то $\varphi \longrightarrow Z/r$ - потенциал ядра. Целесообразно заменить $\varphi(r) = Z\chi(r)/r$ с граничным условием $\chi(0) = 1$.В сферических координатах

$$\Delta\varphi = \frac{1}{r}\frac{d^2}{dr^2}(r\varphi) = \frac{1}{r}\frac{d^2}{dr^2}(Z\chi),$$

следовательно, из (3.37) имеем

$$\frac{Z}{r}\chi''(r) = C\frac{Z^{3/2}}{r^{3/2}}\chi^{3/2},$$

или

$$\chi''(r) = C\frac{Z^{1/2}}{r^{1/2}}\chi^{3/2}.$$

Введем новую переменную $x = \alpha Z^{1/s}$ (α выберем позже) с целью получить универсальное уравнение для функции χ. Тогда из (3.39) находим

$$\alpha^2 Z^{2/3}\chi'' = CZ^{1/2}\frac{1}{x^{1/2}}\alpha^{1/z}Z^{1/a}\chi^{3/2},$$

или, если выбрать $C = \alpha^{3/2}$, т. е. $\alpha = \left(\frac{8\sqrt{2}}{3\pi}\right)^{2/s}$, то окончательно находим

$$\left.\begin{array}{c} \frac{d^2\chi}{dx^2} = \frac{1}{V\bar{x}}\chi^{3/2}, \\ \chi(\infty) = 0, \quad \chi(0) = 1. \end{array}\right\}$$

Уравнение (3.40) решается численно (в 1.1 дано приближенное его решение). Решение его определяет распределение плотности электронов. Характерный радиус этого распределения в безразмерных единицах $x \sim 1$, следовательно, в обычных единицах $a^Z_{\text{Т.-Ф. }\sim a_0/\sqrt[3]{Z}}$. На этом расстоянии находится большинство электронов. Полученный результат совпадает с приближенной оценкой, приведенной на стр. 38. Уравнение (3.40) справедливо в той области атома, где применимо квазиклассическое приближение.

Граница применимости распределения Томаса-Ферми (????)

Начиная с каких и до каких расстояний применимо распределение Томаса - Ферми? (??? не знаю????)

Ответ: $r_{\min} \sim 1/Z, \quad r_{\max} \sim 1.$

(???? а можно конкретно, что не то, если мы на других расстояниях будем его использовать????)

6.6.5 Estimates of Nuclear Matrix Elements

(???? это тренировать еще нужно, не отработал использование этих оценок)

Основные методы

В теории ядра часто приходится вычислять различные суммы матричных элементов. Рассмотрим, какие матричные элементы вносят наибольший вклад в такие суммы.

Пусть $U(r)$ - величина, заметно изменяющаяся на расстояниях порядка радиуса ядра. Оценим квазиклассический матричный элемент $U_{\lambda_1\lambda_2} = (\varphi_{\lambda_1} U \varphi_{\lambda_2})$, где φ_λ - волновая функция нуклона в самосогласованном поле, создаваемом всеми остальными нуклонами ядра, λ - совокупность квантовых чисел, описывающих состояние нуклона.

Рассмотрим сначала сферическое ядро. Тогда $\lambda \equiv n, j, l, m$, где n - радиальное, l - орбитальное и m - магнитное квантовые числа, $j = l \pm \frac{1}{2}$. Покажем, что соседние уровни в сферическом ядре не комбинируют (????) между собой, т. е. дают малое значение матричного элемента $U_{\lambda_1\lambda_2}$.

Предварительно оценим расстояние между соседними уровнями. В деформированном ядре уровни с различными проекциями момента на ось симметрии расщеплены, поэтому если A - число нуклонов в ядре, а ε_F - энергия Ферми, т. е. энергетическое расстояние от дна самосогласованной ямы до места заполнения последних нуклонов, то среднее расстояние между одночастичными уровнями имеет порядок

$$\Delta E \sim \varepsilon_F / A.$$

Величина ε_F не зависит от A с той точностью, с которой постоянна плотность n ядерного вещества. Действительно, в системе, которая удерживается силами, действующими между ее частицами, радиус действия сил и среднее расстояние между частицами имеют одинаковый порядок величины. Поэтому все величины, характеризующие ядро, можно выразить с помощью размерных оценок друг через друга (!???). В частности,

$$\varepsilon_F \sim n^{2/3} \qquad (M = \hbar = 1).$$

В сферическом ядре существует вырождение по проекции углового момента с кратностью порядка величины углового момента

$$l \sim p_F R,$$

где R - радиус ядра, а p_F - импульс нуклона на границе ферми. Так как $R = r_0 A^{1/3}$, где r_0-величина порядка среднего расстояния между нуклонами, то $p_F R = p_F r_0 A^{1/2} \sim A^{1/s}$. Следовательно, среднее расстояние между ближайшими уровнями сферического ядра имеет порядок величины

$$\Delta E \sim \varepsilon_F / A^{2/3}.$$

Расстояние между уровнями с разными радиальными квантовыми числами

Оценим сначала расстояние между уровнями, отличающимися лишь радиальными квантовыми числами n, причем $\delta n \sim 1$. Для этого продифференцируем по n условие квантования Бора $\int p_r dr = n$, где p_r - радиальный импульс. Получаем:

$$1 = \int \frac{\partial p_r}{\partial n} dr = \int \frac{\partial p_r}{\partial \varepsilon_{nl}} \frac{\partial \varepsilon_{nl}}{\partial n} dr \sim \frac{\partial \varepsilon_{nl}}{\partial n} \int \frac{dr}{v} \sim \frac{\partial \varepsilon_{nl}}{\partial n} \frac{R}{v},$$

где ε_{nt} - уровень энергии, а $v = \frac{\partial \varepsilon_{nl}}{\partial p_r}$ - скорость нуклона. Отсюда

$$\frac{\partial \varepsilon_{nt}}{\partial n} \sim \frac{v}{R} = \frac{v}{r_0 A^{1/3}} \sim \frac{p_F v}{A^{1/3}} \sim \frac{\varepsilon_F}{A^{1/3}}.$$

Расстояние между уровнями с разными орбитальными квантовыми числами

Оценим теперь расстояние между уровнями, отличающимися лишь орбитальными квантовыми числами l, причем $\delta l \sim 1$. Для этого продифференцируем по l соотношение $\int p_r dr = n$, учитывая, что $p_r = \sqrt{2\left[\varepsilon_{nl} - V(r) - \frac{(l+1/2)^2}{2r^2}\right]}$.

Здесь $V(r)$-потенциальная энергия нуклона. Получаем:

$$\int \frac{dr}{p_r} \left(\frac{\partial \varepsilon_{nl}}{\partial l} - \frac{l}{r^2} \right) = 0,$$

Т. е.

$$\frac{\partial \varepsilon_{nl}}{\partial l} \int\limits_{r_{\min}}^{R} \frac{dr}{p_r} \sim l \int\limits_{r_{\min}}^{R} \frac{dr}{r^2 p_r},$$

где $r_{\min}$ находится из условия $p_r = 0$, т. е. $r_{\min} \sim l/p_F$. В интеграле $\int\limits_{r_{\min}}^{R} \frac{dr}{p_r}$ существенна вся область интегрирования, поэтому мы его оцениваем как R/v (?? видимо, считаем массу равной 1???). А в интеграле $\int\limits_{r_{\min}}^{R} \frac{dr}{r^2 p_r}$ основной вклад вносится областью вблизи $r_{\min}$, поэтому его оценка $1/(r_{\min} p_F) \sim 1/l$. Итак, $\frac{\partial \varepsilon_{nl}}{\partial l} \cdot \frac{R}{v} \sim l \frac{1}{l} = 1$, т. е.

$$\frac{\partial \varepsilon_{nl}}{\partial l} \sim \varepsilon_F / A^{1/3}.$$

Таким образом, мы получили, что

$$\frac{\partial \varepsilon_{nl}}{\partial n} \sim \frac{\partial \varepsilon_{nl}}{\partial l} \sim \varepsilon_F A^{-1/3}.$$

Поэтому уровень сферического ядра, ближайший к данному, т. е. отстоящий от него на расстоянии $\varepsilon_F/A^{2/3}$, получается, как правило, за счет больших изменений δn и δl, так чтобы величина

$$\delta\varepsilon_{nl} = \frac{\partial\varepsilon_{nl}}{\partial n}\delta n + \frac{\partial\varepsilon_{nt}}{\partial l}\delta l$$

была минимальна. Для этого нужно выбрать $\delta n, \delta l \sim A^{1/3}$. Следовательно, ближайшие уровни сферического ядра, как правило, сильно отличаются по числу узлов радиальной и угловой части волновой функции, а потому дают малое значение матричного элемента $U_{\lambda_1\lambda_3}$.

Состояния с энергнями $|\varepsilon_{\lambda_1} - \varepsilon_{\lambda_2}| \gg \varepsilon_F/A^{1/s}$ также дают малое значение $U_{\lambda_1\lambda_2}$, так как функции $\varphi\lambda_1$ и $\varphi\lambda_2$ сильно различаются по числу узлов.

Итак, матричный элемент $U_{\lambda_1\lambda_2}$ заметно отличен от нуля для $\lambda_1 = \lambda_2$ (если он при этом не равен строго нулю из-за правил отбора) и для $|\varepsilon_{\lambda_1} - \varepsilon_{\lambda_2}| \sim \varepsilon_F A^{-1/3}$, когда числа узлов функций $\varphi\lambda_1$ и $\varphi\lambda_2$ мало различаются.

Об оценках уровней деформированных ядер

Все сказанное выше о комбинирующик (?) уровнях остается в силе и для деформированного ядра, если оператор U меняет квантовые числа n и l. Если же U меняет лишь магнитное квантовое число m (например, оператор углового момента), то комбинируют уровни с соседними m, принадлежащие одному мультиплету nl. Оценим расстояние между ними. Выше (см. стр. 75) было показано, что в первом порядке теории возмущений расщепление уровней определяется соотношением

$$\varepsilon_{ntm} = \varepsilon_{nl} + \varepsilon_{nl}\beta\left(\frac{m^2}{l^2} - \frac{1}{3}\right),$$

где β-величина деформации. Следовательно,

$$\frac{\partial\varepsilon_{ntm}}{\partial m} \sim \varepsilon_{nl}\beta\frac{m}{l^2} \sim \varepsilon_F\beta A^{-1/3},$$

т. е. в этом случае могут комбинировать и близкие уровни (при малых β).

(??? хз, как например это оценивать на практике, ни одного примера не соображу???)

Иллюстрация и примеры оценок в ядерной физике (?????)

(пока не применял этот параграф, потом применю его.)

(??? что-то подозреваю, что у МК бесполезный параграф, потому что с Чармонием задачу нихрена я не могу решить этими формулами. Другую теорию буду писать скорее всего тут еще)

(??? что с Е ферми делать??? мы же не знаем его для ядра??)

Граница применимости таких оценок в ядерной физике (?????)

(??? я хз, для двухчастичных состояний она применима или нет???? мб и нет. не понимаю это пока что.)

Об идее оценивать через $E = mc^2$ и формулу Бора $E_n = -\frac{\alpha}{n^2}$ (???)

(?? хз, так в каких-то вузах предлагают.)

6.6.6 Non-Central Potential (???????)

Основные методы

Рассмотрим более общий случай, когда переменные не разделяются, и построим в этом случае квазиклассическое решение. Ищем решение уравнения

$$\Delta\Psi\Psi + k^2\Psi = 0$$

в виде $\Psi = Ae^{iS}$ Тогда

$$\nabla\Psi = (\nabla A + iA\nabla S)e^{iS},$$

$$\Delta\Psi = \left(\Delta A + 2i\nabla A\nabla S + iA\Delta S - A(\nabla S)^2\right)e^{is}.$$

Следовательно,

$$\Delta A + 2i\nabla A\nabla S - A(\nabla S)^2 + iA\Delta S + k^2 A = 0.$$

Разделяя действительную и мнимую части, из (3.41) получаем два уравнения

$$\Delta A + k^2 A = A(\nabla S)^2,$$

$$2\nabla A\nabla S + A\Delta S = 0.$$

Уравнение $2\nabla A\nabla S + A\Delta S = 0$ означает закон сохранения тока частиц. Действительно,

$$j = \frac{1}{2}\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right) = \frac{1}{2i}\left[Ae^{-iS}\nabla\left(Ae^{iS}\right) - Ae^{iS}\left(\nabla Ae^{-iS}\right)\right] = A^2\nabla S$$

и

$$\operatorname{div} j = \nabla\left(A^2\nabla S\right) = A^2\Delta S + 2\nabla A\nabla S\cdot A = 0.$$

Следовательно, вдоль линии тока

$$j_1 d\sigma_1 = j_2 d\sigma_2,$$

где $d\sigma_1$ и $d\sigma_2$ - нормальные элементы площади трубки тока.

Если $\Delta A/A \ll k^2$, то из $\Delta A + k^2 A = A(\nabla S)^2$ следует уравнение Гамильтона-Якоби для S:

$$2[E - V(r)] = (\nabla S)^2.$$

6.6.7 Quasi-Classical Scattering Problem

Построим квазиклассическую волновую функцию для задачи рассеяния. Гредварительно заметим, что уравнение (3.45) содержит не одно решение: в любую точку в $+\infty$, куда устремляются частицы после рассеяния, частица может прийти по меньшей мере двумя путями. Это изображено на рис. 31.

(??????????? тут рисунок, который я вообще не понимаю)

Здесь 1 и 2 - две точки фронта плоской падающей волны.

Поэтому на основе принципа суперпозиции вместо решения $\Psi = Ae^{iS}$ мы должны потребовать $\Psi = \sum_i A_i e^{iS_l}$, где сумма берется по всем классическим траекториям, соединяющим рассматриваемые точки.

Предположим для простоты, что есть только две траектории, соединяющие фронты падающей и рассеянной волн на бесконечности. Вдоль траектории I, которая 'проходит втали от центра рассеяния, трубка тока параллельна оси x; A и ∇S постоянны, причем

$\nabla S = p_0$. Можно положить, что значение Ц-функции в каждой точке фронта падающей волны равно 1. Поэтому $A_1 = A_2 = 1$. Следовательно,

$$\Psi_1 = \exp\left[i\int\limits_{-L}^{x} p_0 dx\right] = \exp\left(ip_0 x + ip_0 L\right),$$

где L - пока произвольное число. Найдем второе решение Ψ_2. Вдоль второй трубки тока $A^2 \nabla S d\sigma = \text{const}$. На $-\infty$ имеем $A_2 = 1, \nabla S = p_0, d\sigma = \rho d\rho d\varphi$, где ρ - прицельный параметр. Следовательно,

$$p_0 \rho d\rho d\varphi = A_2^2 p_0 r^2 d\Omega.$$

Тогда

$$\Psi_2 \underset{r\to\infty}{\to} A_2 e^{iS_2} = \sqrt{\frac{\rho d\rho d\varphi}{r^2 d\Omega}} \exp\left[i\int\limits_{-L}^{r} pdl\right],$$

а полное решение задачи имеет вид

$$\Psi \underset{r\to\infty}{\to} \exp\left(ip_0 x + ip_0 L\right) + \sqrt{\frac{\rho d\rho d\varphi}{r^2 d\Omega}} \exp\left[i\int\limits_{-L}^{r} pdl\right].$$

Умножим правую часть этого равенства на постоянный множитель $e^{-ip_0 L}$:

$$\Psi \underset{r\to\infty}{\longrightarrow} e^{ip_0 x} + \sqrt{\frac{\rho d\rho d\varphi}{r^2 d\Omega}} \exp i\left[p_0 r + \int\limits_{-L}^{r} pdl - \int\limits_{-L}^{r} p_0 dl - p_0 L\right],$$

или $\Psi \underset{r\to\infty}{\to} e^{ip_0 x} + \frac{f}{r} e^{ip_0 r}$, где $f = \sqrt{\left(\frac{d\sigma}{d\Omega}\right)_{K\pi}} e^{i\Phi}, \Phi \equiv \int\limits_{-\infty}^{\infty} pdl - \int\limits_{-\infty}^{\infty} p_0 dl_0$. Траектории l и l_0 изображены на рис. 32.

(добавлю потом его)

О рассеянии с точками, где квазиклассика неприменима

В выражении (3.49) фактически существенное значение имеют точки вблизи центра рассеяния. Выражение (3.49) требует уточнения в том случае, когда классическаи траектория проходит вблизи точек, где квазиклассика неприменима. Совокупность таких точек образует поверхность, называемую каустикой. Каустика отделяет область, доступную для классического движения, от недоступной. Например, для отталкивательного кулоновского потенцнала каустика имеет вид параболоида враіцения. В случае притягивательного кулоновского потенциала она предстазляет собой прямую линию, идущую от liентра рассеяния к $+\infty$.

Найдем, как меняется фаза волновой функции вблизи касания траектории с каустикой. Разложим движение частицы на два движения: перпендикулярно касательной к каустике и вдоль касательной. Движение в перпендикулярном направлении аналогично квазиклассическому отражению от точки поворота в одномерной задаче. При этом разность фаз падающей н отраженной волны, как мы видели, равна $\pi/4 - (-\pi/4) = \pi/2$. При движении вдоль касательной к каустике изменения фазы не происходит. Следовательно, вместо (3.49) для Φ получается следующее выражение:

$$\Phi = \int\limits_{-\infty}^{\infty} pdl - \int\limits_{-\infty}^{\infty} p_0 dl_0 + iv\frac{\pi}{2},$$

где v - число точек касания с каустикой. В случае кулоновского ногенциала $v = 1$.

Сечение рассеяния протона на атоме водорода

При рассмотрении задачи о перезарядке (см. стр. 103 (???)) было получено, что амплитуда рассеяния $f_1 = 1/2\,(f_s + f_a)$, а амплитуда перезарядки $f_2 = 1/2\,(f_s - f_a)$, где f_s, f_a - амплитуды соответственно симметричного и антисимметричного рассеяния.

Потенциал V_s мало отличается от V_a, поэтому классическое сечение можно считать одинаковым для V_s и V_u, между тем как фазы Φ_s и Φ_a могут сильно различаться. Действительно, $\mathfrak{D}_s, \mathscr{D}_a$ - очень большие числа, поэтому и $\Phi_s - \Phi_a$ может быть велико.

Следовательно, согласно (3.48)

$$f_1 = \frac{1}{2}\sqrt{\left(\frac{d\sigma}{d\Omega}\right)_\pi}\left(e^{i\Phi_s} + e^{i\Phi_a}\right), f_2 = \frac{1}{2}\sqrt{\left(\frac{d\sigma}{d\Omega}\right)_\Omega}\left(e^{i\Phi_s} - e^{i\Phi_a}\right).$$

Сечение перезарядки равно

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{перез}} = |f|^2 = \frac{1}{4}\left(\frac{d\sigma}{d\Omega}\right)_{\text{cl}}\left|e^{i\Phi_s} - e^{i\Phi_a}\right|^2 = \left(\frac{d\sigma}{d\Omega}\right)_{\text{cl}}\sin^2\frac{1}{2}\left(\Phi_s - \Phi_a\right)^\circ.$$

Так как

$$\Phi \equiv \int\limits_{-\infty}^{\infty} pdl - \int\limits_{-\infty}^{\infty} p_0 dl_0$$

то

$$\Phi_s - \Phi_a = \int\limits_{-\infty}^{\infty}\left(p_s - p_a\right)dl \approx \int\limits_{-\infty}^{\infty}\frac{m_1\left(V_s - V_a\right)}{p}dl \approx \frac{1}{v_0}\int\limits_{-\infty}^{\infty}\left(V_s - V_a\right)dl,$$

где m_1 - масса, а v_0 - скорость протона.

Рассеяние на малые углы

Рассмотрим рассеяние на малые углы. Обозначим $V_s - V_a \equiv V$. Тогда для сечения перезарядки получаем следующее выражение:

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{перез}} = \left(\frac{d\sigma}{d\Omega}\right)_{\text{кл}}\sin^2\left[\frac{1}{2v_0}\int\limits_{-\infty}^{\infty} V\left(\sqrt{\rho^2 + x^2}\right)dx\right],$$

Здесь ρ - прицельный параметр. Это выражение совпадает с сечением, полученным в (2.4). Для сечения рассеяния получаем

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{расс}} = \left(\frac{d\sigma}{d\Omega}\right)_{\text{кл}}\cdot\cos^2\left[\frac{1}{2v_0}\int\limits_{-\infty}^{\infty} V\left(\sqrt{\rho^2 + x^2}\right)dx\right] =$$

$$= \frac{1}{2}\left(\frac{d\sigma}{d\Omega}\right)_{\text{кл}} - \frac{1}{2}\left(\frac{d\sigma}{d\bar{\Omega}}\right)_{\text{кл}}\cdot\cos\left[\frac{1}{v_0}\int\limits_{-\infty}^{\infty} V\left(\sqrt{\rho^2 + x^2}\right)dx\right].$$

Таким образом, наряду с обычным классическим рассеянием получаются квантовомеханические осцилляции сечения рассеяния как функции угла отклонения.

6.7 Adiabatic methods

Обсудим подробно адиабатические методы.

6.7.1 Non-stationary Adiabatics

Statement of the problem in scope of non-stationary adiabatics

Пусть гамильтониан системы адиабатически - очень медленно - меняется во времени, $\hat{H} = \hat{H}(t)$. Мы будем интересоваться тем, как устроено решение нестационарного уравнения Шрёдингера:

$$i\frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$$

В принципе адиабатичность изменения параметров подразумевает предельный случай - параметры меняются бесконечно медленно.

Естественно, в реальных задачах бесконечно медленно параметры менять невозможно, и поэтому всегда имеется некий характерный масштаб времени T, определяющий скорость изменения параметров, и адиабатичность означает, что этот масштаб времени - большой. Но с чем его нужно сравнивать? Для этого предлагается привлечь интуицию, приходящую от нестационарной теории возмущений. Если имеется возмущение, которое зависит от времени периодически, то имеются переходы между состояниями, причём состояния разнесены по энергии на ω -частоту этого возмущения. Всякое непериодическое возмущение, в свою очередь, можно расписать в интеграл Фурье и представить как комбинацию периодических; в нашем случае, характерные частоты преобразования Фурье определяются из соотношения неопределённостей, $\omega \sim \frac{1}{T}$ (тем самым, частоты очень маленькие).

Теперь можно более чётко сформулировать критерий адиабатичности: частоты должно быть недостаточно для обеспечения переходов,

$$\omega \ll \Delta E \to T \gg \frac{1}{\Delta E},$$

where ΔE -типичное расстояние между соседними уровнями энергии системы, level spacing.

Уровни энергии в случае гамильтониана, зависяшего от времени - понятие бессмысленное, но если мы имеем дело с адиабатикой, то подразумеваются мгновенные уровни энергии гамильтониана - диагонализация гамильтониана в каждый конкретный момент времени:

$$\hat{H}(t)|n(t)\rangle = E_n(t)|n(t)\rangle$$

Ещё раз подчеркнём, что $|\psi_n(t)\rangle$ ни в коем случае не являются решениями нестационарного уравнения Шурёдингера! (?????? why?????)

Пусть теперь в начальный момент времени $t = 0$ мы «посадили» частицу в одно из собственных состояний гамильтониана $|\psi(0)\rangle = |\psi_n(0)\rangle$. Вышеприведённые рассуждения позволяют нам заключить, что в адиабатическом пределе $T \to \infty$ состояние системы в произвольный момент времени t будет $|\psi(t)\rangle \propto |\psi_n(t)\rangle$ (с точностью до фазового множителя) то есть волновая функция будет следовать мгновенному состоянию данного гамильтониана. This is the main philosophy of adiabatic method.

Это утверждение напрямую связано с сохранением адиабатического инварианта в классической механике. (??? see quasiclassics, why???)

We also assume that change of the energy level is occurring after the evolution. Not like a particle can be measured ones it locates at a new level. This is the big question about measurement, and we are not touching it here. Change of the state in scope of the adiabatic method happens only by change of coefficients and this is what we are dealing with. Thus it is only an approximate method for toy models and in real life, there are a lot of interactions in the intermediate dynamics which are not taken into account.

Derivation of general formulas of non-stationary adiabatics

Выведем все нужные формулы нестационарной адиабатики.

Поскольку мгновенные собственные состояния гамильтониана образуют базис, разложим волновую функцию: $|\psi(t)\rangle = \sum\limits_m \psi_m(t)\,|m(t)\rangle$, подставим в уравнение Шрёдингера:

$$i\partial_t \sum_m \psi_m(t)\,|m(t)\rangle = \sum_m E_m(t)\psi_m(t)\,|m(t)\rangle$$

$$i\sum_m \left(\partial_t\psi_m(t)|m(t)\rangle + \psi_m(t)\partial_t|m(t)\rangle\right) = \sum_m E_m(t)\psi_m(t)|m(t)\rangle.$$

Подставим

$$\psi_m(t) = c_m(t)\cdot\exp\left(-i\int\limits_{t_0}^{t} E_m(\tau)d\tau\right),$$

где $\int\limits_{t_0}^{t} E_n(\tau)d\tau$ - так называемая динамическая фаза.

(why exactly we substitute this? answer is in the derivation below, but I'd like to also write words)

Получим

$$i\sum_m\left(\partial_t\left[c_m(t)e^{\left(-i\int\limits_{t_0}^{t}E_m(\tau)d\tau\right)}\right]|m(t)\rangle + c_m(t)e^{\left(-i\int\limits_{t_0}^{t}E_m(\tau)d\tau\right)}\partial_t|m(t)\rangle\right) =$$

$$=i\sum_m\left(\partial_t c_m(t)\cdot e^{-i\int\limits_{t_0}^{t}E_m(\tau)d\tau}|m(t)\rangle + c_m(t)\partial_t e^{-i\int\limits_{t_0}^{t}E_m(\tau)d\tau}|m(t)\rangle + c_m(t)e^{-i\int\limits_{t_0}^{t}E_m(\tau)d\tau}\partial_t|m(t)\rangle\right) =$$

$$=i\sum_m \partial_t c_m(t)\cdot e^{-i\int\limits_{t_0}^{t}E_m(\tau)d\tau}|m(t)\rangle + \sum_m E_m(t)c_m(t)e^{-i\int\limits_{t_0}^{t}E_m(\tau)d\tau}|m(t)\rangle +$$

$$+ i\sum_m c_m(t)e^{\left(-i\int\limits_{t_0}^{t}E_m(\tau)d\tau\right)}\partial_t|m(t)\rangle \equiv$$

$$\equiv \sum_m E_m(t)c_m(t)e^{\left(-i\int\limits_{0}^{t}E_m(\tau)d\tau\right)}|m(t)\rangle.$$

Сокращаем слагаемое справа с одним из левой части, получаем уравнение:

$$i\sum_m \partial_t c_m(t)\cdot e^{\left(-i\int\limits_{t_0}^{t}E_m(\tau)d\tau\right)}|m(t)\rangle + i\sum_m c_m(t)e^{\left(-i\int\limits_{t_0}^{t}E_m(\tau)d\tau\right)}\partial_t|m(t)\rangle = 0$$

Спроецируем на бра-вектор $\langle n(t)|$, и пользуясь $\langle n(t)|m(t)\rangle = \delta_{nm}$, получим

$$i\partial_t c_n(t)\cdot e^{\left(-i\int\limits_{t_0}^{t}E_n(\tau)d\tau\right)} + i\sum_m c_m(t)e^{\left(-i\int\limits_{t_0}^{t}E_m(\tau)d\tau\right)}\langle n(t)\partial_t|m(t)\rangle = 0,$$

тогда окончательно

$$\frac{dc_n(t)}{dt} = -\sum_m c_m(t)e^{-i\int\limits_{t_0}^{t}\omega_{mn}(\tau)d\tau}\langle n(t)\partial_t|m(t)\rangle,$$

где введено стандартное обозначение $\omega_{mn} = E_m - E_n$.

Правая часть этого уравнения мала. она содержит производные по времени мгновенного базиса, который меняется на больших временных масштабах $t \sim T$. (?? check!!!) Поэтому это уравнение уже приспособлено для решения его методом последовательных приближений.

Пусть в начальный момент времени мы находились в каком-то состоянии $|n\rangle$, то есть $c_n(0) = 1$. Найдем амплитуду перехода в $|m\rangle$ за конечное время $c_m(t)$, где $m \neq n$.

Приведём наивную оценку, которая продемонстрирует явно, что $c_m(t)$ мал в меру адиабатичности. Для оценки $\left(\sum_m c_m(t) e^{-i\int_{t_0}^{t} \omega_{mn}(\tau)d\tau} \langle n(t)\partial_t|m(t)\rangle \right)$ продифференцируем по t уравнение $\hat{H}(t)|m(t)\rangle = E_m(t)|m(t)\rangle$, спроецируем его на $\langle n(t)|$ и воспользуемся $\langle n(t)|m(t)\rangle = \delta_{nm}$:

$$\partial_t \hat{H} \cdot |m(t)\rangle + \hat{H}\partial_t|m(t)\rangle = \partial_t E_m|m(t)\rangle + E_m\partial_t|m(t)\rangle$$

$$\langle n(t)|\partial_t\hat{H}|m(t)\rangle + (\langle n(t)|\hat{H})\partial_t|m(t)\rangle = \partial_t E_m\langle n(t)|m(t)\rangle + E_m\langle n(t)|\partial_t|m(t)\rangle$$

$$\langle n(t)|\partial_t\hat{H}|m(t)\rangle = \partial_t E_n\delta_{nm} + (E_m(t) - E_n(t))\,\langle n(t)\,|\partial_t|\,m(t)\rangle$$

получим:

$$\langle n(t)\,|\partial_t|\,m(t)\rangle = -\frac{\langle n(t)|\partial_t\hat{H}|m(t)\rangle}{\omega_{nm}(t)}, \quad m \neq n$$

Производная гамильтониана уже явно содержит параметр $1/T$ (!?! укажу про это выше), а в знаменателе оказался level spacing ω_{nm}, поэтому

$$\left(\sum_m c_m(t) e^{-i\int_{t_0}^{t} \omega_{mn}(\tau)d\tau} \langle n(t)\partial_t|m(t)\rangle \right) \sim \frac{1}{\omega_{nm}T} \ll 1.$$

(потом еще про это подумаю, пока не полностью владею такими оценками.)

First order approximation of non-stationary adiabatics

So, at this moment we are developing formulas for a general problem

$$i\frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle.$$

We decomposed the functions into basis vectors $|\psi(t)\rangle = \sum_m \psi_m(t)\,|m(t)\rangle$, and each coefficient of the decomposition, we parameterize by $c_m(t)$ as

$$\psi_m(t) = c_m(t) \cdot \exp\left(-i\int_{t_0}^{t} E_m(\tau)d\tau \right).$$

we got that they are changing according to

$$\frac{dc_n(t)}{dt} = -\sum_m c_m(t) e^{-i\int_{t_0}^{t} \omega_{mn}(\tau)d\tau} \langle n(t)\partial_t|m(t)\rangle.$$

Рассматривая теперь ведущее приближение для $c_m(t)$, оставим только один член в этой формуле. This is a very important approximation.

(???? why other states m in the formula $\sum_m$ will give much less contribution. Currently I don't see it.)

Now, we substitute $\langle n(t)\,|\partial_t|\,m(t)\rangle = -\frac{\langle n(t)|\partial_t \hat{H}|m(t)\rangle}{\omega_{nm}(t)}$ and get

$$c_m(T) \approx \int\limits_{t_0}^{T} \exp\left(i\int\limits_{t_0}^{t}\omega_{mn}(\tau)d\tau\right)\frac{\left\langle m(t)\left|\partial_t\hat{H}\right|n(t)\right\rangle}{\omega_{mn}(t)}dt,$$

where $|n(t)\rangle$ is the only one state to which particle can travel. Это выражение, в действительности, представляет собой интеграл типа «медленная огибающая на быстроосциллирующий фактор». Такого рода интегралы, как правило, содержат экспоненциальную малость, что мы и продемонстрируем на примере следующей задачи.

So, totally, we can work with adiabatic methods with equation with $\partial_t|m(t)\rangle$ or with $\partial_t\hat{H}$. It depends on what is more comfortable.

Задача Ландау-Зенера методами нестационарной адиабатики

Обсудим задачу Ландау-Зенера как типичный пример нестационарной адиабатики. Поскольку параметр адиабатичности $\frac{1}{\omega_{nm}T} \ll 1$ явно содержит level spacing $\omega_{nm} = \omega_{nm}(t)$, больше всего переходы между различными состояниями будут происходить, между парой уровней, которые максимально сближаются. Поэтому такую ситуацию можно сформулировать в достаточно общем виде как чисто двухуровневую задачу. Такая задача носит название задачи Ландау-Зенера, и описывается следующим гамильтонианом:

$$\hat{H}(t) = \begin{pmatrix} \alpha t & \gamma \\ \gamma & -\alpha t \end{pmatrix}$$

Задача Ландау-Зенера адиабатическим методом

Для системы с

$$\hat{H}(t) = \begin{pmatrix} \alpha t & \gamma \\ \gamma & -\alpha t \end{pmatrix}$$

Найдем мгновенные собственные состояния:

$$E_+(t) = \sqrt{\gamma^2+(\alpha t)^2}, \qquad |\psi_+(t)\rangle = \frac{1}{\sqrt{2\left(\gamma^2+(\alpha t)^2+\alpha t\sqrt{\gamma^2+(\alpha t)^2}\right)}}\begin{pmatrix} \alpha t+\sqrt{\gamma^2+(\alpha t)^2}\end{pmatrix}\\ \gamma \end{pmatrix}$$

$$E_-(t) = -\sqrt{\gamma^2+(\alpha t)^2}, \quad |\psi_-(t)\rangle = \frac{1}{\sqrt{2\left(\gamma^2+(\alpha t)^2-\alpha t\sqrt{\gamma^2+(\alpha t)^2}\right.}}\begin{pmatrix} \alpha t-\sqrt{\gamma^2+(\alpha t)^2} \\ \gamma \end{pmatrix}$$

(Check it!)

We introduce $\alpha t = \gamma\sinh\theta$ and get:

$$E_+(\theta) = \gamma\cosh\theta, \qquad |\psi_+(\theta)\rangle = \frac{1}{\sqrt{2\cosh\theta}}\begin{pmatrix} e^{\theta/2} \\ e^{-\theta/2}\end{pmatrix}$$

$$E_-(\theta) = -\gamma\cosh\theta, \qquad |\psi_-(\theta)\rangle = \frac{1}{\sqrt{2\cosh\theta}}\begin{pmatrix} e^{-\theta/2} \\ -e^{\theta/2}\end{pmatrix}$$

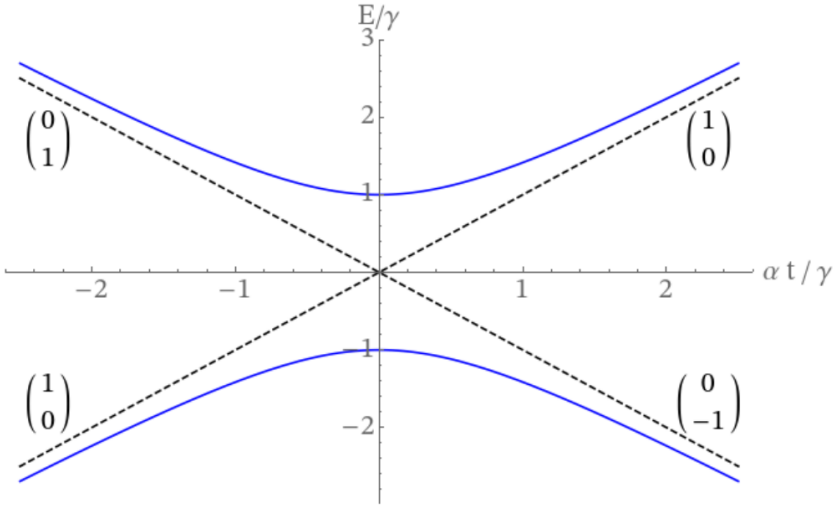


Figure 6.4: Уровни в задаче Ландау-Зенера (?? I think, here it it typo, there should not be -1 at the low part)

Пусть в момент времени $t \to -\infty$ мы находились на верхней ветке, то есть $|\psi_+(-\infty)| = 1$ и $|\psi_-(-\infty)| = 0$. Note that here ψ-s are coefficients in the original basis, where the Hamiltonian is not diagonal. Мы интересуемся вероятностью перехода в результате адиабатической эволюции на нижнюю ветку, которая определяется по формуле

$$P = |\psi_-(+\infty)|^2 .$$

Proof.

$$P = |\langle\downarrow||\psi(+\infty)\rangle|^2 = |(\langle\downarrow|)(\psi_-(+\infty)|\downarrow\rangle + \psi_+(+\infty)|\uparrow\rangle)|^2 = |\psi_-(+\infty)|^2$$

so it is equal to this coefficient.

□

Выделим параметр адиабатичности $\frac{1}{\omega_{nm}T} \ll 1$. Если уровни находятся достаточно далеко по энергии, то переходов не будет - поэтому масштаб времени T, который входи't в критерий адиабатичности, определяется из условия достаточной близости уровней: $\alpha T \sim \gamma \to T \sim \frac{\gamma}{\alpha}$. С другой стороны, масштаб расстояния между уровнями при этом равен γ. Поэтому адиабатическое приближение соответствует случаю, когда $\gamma^2 \gg \alpha$

(??? Think about this more!!)

We use $c_m(T) \approx \int\limits_{t_0}^{T} \exp\left(i \int\limits_{t_0}^{t} \omega_{mn}(\tau)d\tau\right) \frac{\langle m(t)|\partial_t \hat{H}|n(t)\rangle}{\omega_{mn}(t)} dt$ for our case:

$$c_+(+\infty) = \int\limits_{-\infty}^{\infty} \exp\left(i \int\limits_{0}^{\theta} \omega_{+-}(\theta)\frac{d\tau}{d\theta}d\theta\right) \frac{\left\langle \psi_+ \left| \partial_\theta \hat{H} \right| \psi_- \right\rangle}{\omega_{+-}(\theta)} d\theta$$

(??! про переход к параметру еще подумаю.)

Здесь:

$$\partial_\theta \hat{H} = \gamma \begin{pmatrix} \cosh\theta & 0 \\ 0 & -\cosh\theta \end{pmatrix}$$

$$\langle\psi_+|\partial_\theta \hat{H}|\psi_-\rangle = \gamma$$

(!??! ниже не додумывал математику, потом еще раз проверю.)

Входящие сюда искомые величины равны:

$$\langle\psi_-(\theta)\left|\frac{\partial\hat{H}}{\partial\theta}\right|\psi_+(\theta)\rangle = \frac{1}{2\cosh\theta}\left(e^{-\theta/2}-e^{\theta/2}\right)\begin{pmatrix}\gamma\cosh\theta & 0\\ 0 & -\gamma\cosh\theta\end{pmatrix}\begin{pmatrix}e^{\theta/2}\\ e^{-\theta/2}\end{pmatrix} = \gamma$$

и

$$\int\limits_0^t \omega_{+-}(\tau)d\tau = 2\frac{\gamma^2}{\alpha}\int\limits_0^\theta \cosh^2\theta d\theta = \frac{\gamma^2}{\alpha}\left[\theta+\frac{1}{2}\sinh 2\theta\right]$$

и искомая амплитуда даётся интегралом:

$$c_-^{(1)}(\infty) = \int\limits_{-\infty}^{\infty}\frac{\exp\left(-i\frac{\gamma^2}{\alpha}\left(\theta+\frac{1}{2}\sinh 2\theta\right)\right)}{2\cosh\theta}d\theta$$

Вычисление интеграла для численного ответа.

(пока так и не тренировал и не смотрел.)
Вычислим

$$c_-^{(1)}(\infty) = \int\limits_{-\infty}^{\infty}\frac{\exp\left(-i\frac{\gamma^2}{\alpha}\left(\theta+\frac{1}{2}\sinh 2\theta\right)\right)}{2\cosh\theta}d\theta.$$

Перед нами - классический пример интеграла вида «быстро-осциллирующая функция + медленная огибающая». Интегралы такого вида берутся методом стационарной фазы, или более общо - методом перевала. В данном конкретном случае, фаза $f(\theta)=\theta+\frac{1}{2}\sinh 2\theta$ и $f'(\theta)=1+\cosh 2\theta\geq 2$, поэтому точек стационарной фазы на вещественной оси нет. Тут мы не будем гоняться за точностью оценки, а выделим лишь ведущую экспоненциальную асимптотику интеграла. Для этого мы можем сделать так, чтобы в экспоненте стояла линейная функция, перейдя к интегралу по $z=\theta+\frac{1}{2}\sinh 2\theta \to dz = d\theta(1+\cos 2\theta) = 2\cosh^2\theta d\theta$, и переписав интеграл в виде:

$$c_-^{(1)}(\infty) = \int\limits_{-\infty}^{\infty}\frac{\exp\left(-i\frac{\gamma^2}{\alpha}z\right)}{4\cosh^3\theta}dz$$

Теперь мы можем применить лемму Жордана, замкнув контур интегрирования в нижней полуплоскости (где экспонента затухает), и сведя его к вычетам в полюсах, которые определяются из уравнения $\cosh\theta=0\to\theta_k=-i\frac{\pi}{2}(1+2k)=z_k$. Беря только полюс с $k=0$, и оставляя только экспоненту, мы получаем ответ:

$$c_-^{(1)}(\infty)\sim e^{-\pi\gamma^2/2\alpha}\to P\sim e^{-\pi\gamma^2/\alpha}$$

Comments about Landau-Zener problem

- Во-первых, ответ получился экспоненциально мал, что и обосновывает адиабатическое приближение. Действительно, переходы в другие состояния практически отсутствуют! Это утверждение весьма общего характера: глядя на уравнение $i\partial_t c_n(t) = -i\sum_m \exp\left(i\int_{t_0}^t\omega_{nm}(\tau)d\tau\right)\langle n(t)|\partial_t|m(t)\rangle c_m(t)$, мы понимаем, что поправка всегда будет устроена как быстро-осциллирующая функция (связанная с динамической фазой) + медленная огибающая (связанная с медленной зависимостью мгновенных

стационарных волновых функций), а интегралы такого вида, как правило, действительно содержат экспоненциальную малость.

(???)

- Во-вторых, следует сделать комментарий по поводу того, почему мы не стали оценивать предэкспоненту. Дело в том, что если сделать вторую итерацию адиабатического приближения, то поправка окажется малой с той же экспонентой и не будет содержать малости по сравнению с первой. В данном случае это означает, что адиабатическое приближение позволяет правильно определить показатель экспоненты, но предэкспонента находится за пределами её точности.

(????)

- В-третьих, показатель экспоненты в более или менее общем виде можно определить, используя метод перевала. Действительно, для этого достаточно определить комплексную точку перевала, условие на которую, в действительности, очень просто: $\omega_{mn}(t_0) = 0$ (в нашем случае это соответствует $t = -i\frac{\gamma}{\alpha}$), и тогда вероятность перехода дастся интегралом $P \sim \exp\left(-2\,\mathrm{Im}\int^{t_0}\omega_{mn}(t)dt\right)$

Более того, точно такое же выражение возникает при изучении вопроса о сохранении адиабатического инварианта в классической механике, что подчёркивает сходство этих двух задач.

- Наконец, as it is well-known, задача Ландау-Зенера решается абсолютно точно и без адиабатического приближения, и ответ в ней оказывается точно равен этой экспоненте: $P = e^{-\pi\gamma^2/\alpha}$.

Описание геометрии для нестационарной адиабатики (!?)

(на это есть задачи, важная идея, потом опишу.)

6.7.2 Non-stationary Adiabatics by Migdal Krainov

Теория

В этом разделе рассматривается случай, когда возмущение, действуюшее на квантовомеханическую систему, медленно меняется со временем. При этом система успевает псрестраиваться вслед за медленным изменением параметров. Такие возмушения называюотся адиабатическими.

В случае адиабатических возмущений удобно искать решение уравнения Шредингера в виде суперпозиции стационарных собственных функций, вычисленных при произвольных, но фиксированных значениях параметров.

Предположим, что гамильтониан $H(x,\xi)$ зависит от медленно меняющегося параметра ξ. Введем собственныс фугкции $\varphi_m(x,\xi)$ гамильтониана $H(x,\xi)$, в которых значение ξ зафик сировано:

$$H(x,\xi)\varphi_m(x,\xi) = \varepsilon_m(\xi)\varphi_m(x,\xi).$$

Будем искать решение уравнения Ц иедингера

$$i\frac{\partial\Psi}{\partial t} = H\Psi$$

В виде

$$\Psi = \sum_m a_m(t)\varphi_m(x,\xi)\exp\left\{-i\int\limits_{-\infty}^{t}\varepsilon_m(\xi)dt\right\}$$

Подставляя (2.25) в (2.24), находим

$$i\sum_m \exp\left\{-i\int\limits_{-\infty}^{t}\varepsilon_m(\xi)dt\right\}\left(\tfrac{da_m}{dt} - i\varepsilon_m a_m + a_m\xi\tfrac{\partial}{\partial\xi}\right)\varphi_m(x,\xi) =$$

$$= \sum_m \exp\left\{-i\int\limits_{-\infty}^{t}\varepsilon_m(\xi)dt\right\}\varepsilon_m\varphi_m(x,\xi),$$

откуда

$$\tfrac{da_n}{dt} + \sum_m\left(\varphi_n|\tfrac{\partial\varphi_m}{\partial\xi}\right)\dot\xi a_m\exp\left\{-i\int\limits_{-\infty}^{t}(\varepsilon_m-\varepsilon_n)\,dt\right\} = 0.$$

Уравнение (2.26) эквивалентно исходному Уравнению Шредингера (2.24). В отличие от (2.24), оно удобно для нахождения последовательных приближений при малых???? Именно,

$$a_n^{(0)}(t) = a_n(-\infty),$$

$$a_n^{(1)}(t) = -\int\limits_{-\infty}^{t}dt'\sum_m\left(\varphi_n|\frac{\partial\varphi_m}{\partial\xi}\right)\xi\times a_m(0)\exp\left\{-i\int\limits_{-\infty}^{t'}(\varepsilon_m-\varepsilon_n)\,dt'\right\}$$

Н Т. д. Выразим $\left(\varphi_n|\frac{\partial\varphi_m}{\partial\xi}\right)$ через матричный элемент гамильтониана H. Дифференцируя соотношение (2.23) по параметру?, находим

$$\frac{\partial H}{\partial\xi}\varphi_m + H\frac{\partial\varphi_m}{\partial\xi} = \frac{d\varepsilon_m}{d\xi}\varphi_m + \varepsilon_m\frac{d\varphi_m}{d\xi}$$

Умножая это равенство на φ_n слева и интегрируя по $\boldsymbol{x}$, получаем

$$\left(\varphi_n\left|\frac{\partial H}{\partial\xi}\right|\varphi_m\right) + \varepsilon_n\left(\varphi_n|\frac{\partial\varphi_m}{\partial\xi}\right) = \frac{d\varepsilon_m}{d\xi}\delta_{nm} + \varepsilon_m\left(\varphi_n|\frac{\partial\varphi_m}{\partial\xi}\right).$$

откуда

$\left(\varphi_n|\frac{\partial\varphi_m}{\partial\xi}\right)_{n\neq m} = \frac{\left(\varphi_n\left|\frac{\partial H}{\partial\xi}\right|\varphi_m\right)}{\varepsilon_m-\varepsilon_n}$, $\left(\varphi_n\left|\frac{\partial H}{\partial\xi}\right|\varphi_n\right) = \frac{d\varepsilon_n}{d\xi}$. Будем предполагать, что собственные состояния φ_n не вырождены. Тогда волновые функции φ_n можно выбрать вещественными, и, следовательно, диагоналыный матричный элемент

$$\left(\varphi_n|\frac{\partial\varphi_n}{\partial\xi}\right) = \frac{1}{2}\frac{\partial}{\partial\xi}\int\varphi_n^2 dr = 0.$$

Подставляя (2.28) в (2.27), получаем

$$a_n^{(1)}(t) = -\int\limits_{-\infty}^{t}dt'\sum_m\frac{\left(\varphi_n\left|\frac{\partial H}{\partial\xi}\right|\varphi_m\right)\dot\xi}{\varepsilon_m-\varepsilon_n}\times a_m(-\infty)\exp\left\{-i\int\limits_{-\infty}^{t'}(\varepsilon_m-\varepsilon_n)\,dt'\right\}.$$

Штрих в сумме по m означает, что в него нет диагональных членов.

Критерий применимости адиабатической теории возмущений состоит в том, чтобы изменение гамильтониана за время порядка обратных частот системы было малым по сравнению с энергиями, соответствующими этим частотам.

Критерий применимости легко получить, если оценить отношение поправки $a_n^{(2)}(t)$ к амплитуде $a_n^{(1)}(t)$: учитывая (2.29), находнм

$$\frac{a_n^{(2)}}{a_n^{(1)}} \sim \frac{\partial H}{\partial t} \frac{1}{(\varepsilon_m - \varepsilon_n)^2}.$$

Как видно из (??), отдельного рассмотрения требует случай, когда при некоторых значениях параметров ξ уровни энергии пересекаптся. В этом случае волновую функцию следует искать в виде суперпозиции состояний, соответствующих этим пересекающимся термам.

Покажем, что если обратные собственные частоты систе.мы ω_{mn}^{-1} много меньше временн τ, которое существенно изменяется гамильтониан системы, то эта система, как правило, будет возбуждаться эксионенциально слабо. Действительно, выражение (2.29) для амплитуды персхода $a_n^{(1)}(t)$ сводитсл к фурье-компонентам от функций $\frac{\left(\varphi_n \left| \frac{\partial H}{\partial \xi} \right| \varphi_m\right)\dot{\xi}}{\varepsilon_n - \varepsilon_m}$.

Ранее (см, 1.1) мы видели, что такие фурье- компоненты при $\omega_{mn}\tau \geqslant 1$ экспоненциально малы ($\sim e^{-\omega_{m\mathrm{I}math}\tau}$), ссли Эти функции или их производные не имеют особенностей fa велественной оси.

Как мы видели (см. стр. 53), кулоновские волновые функции имеют особенности на вещественной оси. Поэтому, иапример, вероптиость ионизации атома пролетающей медленной частицей мала степенным образом, а не экспоненциальнО.

MK-ch2.4.1

Используя соотношение (2.28), вычислить $\frac{\bar{1}}{r^2}$ для центральио-симметричного движения.

О т в е т.

$$\frac{T}{r^2} = \frac{1}{l++^1/2} \left(\frac{\partial E}{\partial l}\right)_{n_r}.$$

Захват электрона протоном (перезарядка)

Применим адиабатическуго теориоо возмуцений к задаче о перезарядке при пролете мелленного протона мимо атома водорода. Предположим, что скорость протона много меньше атомнон скорости. Тогда можно применять адиабатнческое прибпижжение.

Кроме того, предположим, что энергия налетающего протона много больше атомной. Тогда можно считать движение гротона заданным.

Гамильтониан системы имеет вид

$$H = T_e - \frac{1}{\left|r - \frac{1}{2}R\right|} - \frac{1}{\left|r + \frac{1}{2}R\right|} + \frac{1}{R}$$

где R - расстоянис между протонами, которое мы будем считать заданной функцией времени; r-координата электрона, T_e - кинетическая энергия электрона.

Гамильтониан H симметричен относительно перестановки налетающего и покоящегося протонов. Такая перестановка эквивалентиа замене $\boldsymbol{r} \longrightarrow - \longrightarrow$. Следовательно, можно ввести синметричные и антисимметричные относительно этой перестановкı соственные функции гамильтониана H : $\varphi_n^s(r,R)$ и $\varphi_n^a(r,R)$. Будем считать, что сначала электрон находился около протона, имеющего координату $R/2$. Тогда волновая функция электрона имеет вид

$$\varphi = \varphi_{n_0}^Q \left(r - \frac{1}{2}R\right),$$

где $\varphi^Q_{n_0}$ - кулоновская волновая функция для состояния n_0.

После рассеяния атом водорода с большой вероятностью останется в состоянии $\varphi^Q_{n_0}$. Действительно, для возбуждения нужна компонента Фурье с частотой, равной энергии возбуждения, $\omega_{nn_0} = \varepsilon_n - \varepsilon_{n_0}$. При медленном пролете, когда время пролета велико по сравнению с обратной частотой $\omega^{-1}_{nn_0}$, компонента Фурье с частотой ω_{nn_0} очень мала и возбуждения не происходит.

Однако электрон может перейти к другому протону. Это явление называется перезарядкой. Критерий адиабатичности (2.30) здесь не выполняется. В самом деле, когда протоны находятся на большом расстоянии друг от друга, волновая Функция электрона равна $\varphi^Q_{n_\bullet}\left(r - \frac{1}{2}R\right)$, если он находится у одного протона, и $\varphi^Q_{n_0}\left(r + \frac{1}{2}R\right)$, - если у другого. Из этих двух функций можно составить симметричную п антисимметричную комбинации $\varphi^s_{n_0}$ и $\varphi^a_{n_0}$. Оба состояния отвечают одной и той же энергии. Следовательно, мы имеем дело с пересечением уровней.

Поэтому решение уравнения Шредингера

$$i\frac{\partial \Psi}{\partial t} = H\Psi$$

следует искать в виде суперпозиции этих двух состояний $\varphi^s_{n_0}$ и $\varphi^a_{n_0}$, после чего нужно применять адиабатическую теорию возмущений. Итак,

$$\Psi = C^s(t)\varphi^s_{n_0}(\boldsymbol{r}, \boldsymbol{R}) \exp\left(-i\int\limits_{-\infty}^{t} \varepsilon^s dt\right) + C^a(t)\varphi^a_{n_0}(\boldsymbol{r}, R) \exp\left(-i\int\limits_{-\infty}^{t} \varepsilon^a dt\right).$$

Подставляя (2.32) в (2.31), получаем

$$\left\{\frac{dC^s}{dt}\varphi^s_{n_0}(\boldsymbol{r}, R) + C^s\frac{dR}{dt}\frac{\partial \varphi^s_{n_0}(\boldsymbol{r}, R)}{\partial R}\right\} \exp\left(-i\int\limits_{-\infty}^{t} \varepsilon^s dt\right) +$$

$$+ \left\{\frac{dC^a}{dt}\varphi^a_{n_0}(\boldsymbol{r}, R) + C^a\frac{dR}{dt}\frac{\partial \varphi^a_{n_0}(\boldsymbol{r}, R)}{\partial R}\right\} \exp\left(-i\int\limits_{-\infty}^{t} \varepsilon^a dt\right) = 0.$$

(2.33)

Умножим (2.33) на $\varphi^s_{n_0}$ и проинтегрируем по координате $\boldsymbol{r}$, пользуясь ортогональностью функций $\varphi^s_{n_0}$ и $\varphi^a_{n_0}$:

$$\left\{\frac{dC^s}{dt} + C^s\frac{dR}{dt}\left(\varphi^s_{n_0}|\frac{\partial \varphi^s_{n_0}}{\partial R}\right)\right\} \exp\left(-i\int\limits_{-\infty}^{t} \varepsilon^s dt\right) = -C^a\frac{dR}{dt}\left(\varphi^s_{n_0}|\frac{\partial \varphi^a_{n_0}}{\partial R}\right) \exp\left(-i\int\limits_{-\infty}^{t} \varepsilon^a dt\right).$$

Если нуклоны находятся далеко друг от друга, то

$$\varphi^{s,a}_n(\boldsymbol{r}, \boldsymbol{R}) \underset{R\to\infty}{\longrightarrow} \frac{1}{\sqrt{2}}\left[\varphi^Q_n\left(r - \frac{1}{2}R\right) \pm \varphi^Q_n\left(r + \frac{1}{2}R\right)\right].$$

Учитывая (2.35), из (2.34) в нулевом приближении получаем

$$C^s = C^s(t = -\infty) = \frac{1}{\sqrt{2}}, \quad C^a = C^a(t = -\infty) = \frac{1}{\sqrt{2}}$$

(это соответствует электрону, находящемуся в момент времени у протона с координатой $R/2$).

При этих значениях C^s, C^a из (2.32) получаем

$$\Psi|_{t\to\infty} = \frac{1}{\sqrt{2}} \exp\left(-i\int\limits_{-\infty}^{\infty} \varepsilon^s dt\right) \times$$
$$\times \frac{\varphi^Q_{n_0}\left(r-\frac{1}{2}R\right)+\varphi^Q_{n_0}\left(r+\frac{1}{2}R\right)}{V\overline{2}} + \frac{1}{\sqrt{2}} \exp\left(-i\int\limits_{-\infty}^{\infty} \varepsilon^a dt\right) \times$$
$$\times \frac{\varphi^Q_{n_0}\left(r-\frac{1}{2}R\right)-\varphi^Q_{n_0}\left(r+\frac{1}{2}R\right)}{\sqrt{2}} = \frac{1}{2}\left(\exp\left(-i\int\limits_{-\infty}^{\infty} \varepsilon^s dt\right) + \right.$$
$$\left. + \exp\left(-i\int\limits_{-\infty}^{\infty} \varepsilon^a dt\right)\right) \varphi^Q_{n_0}\left(r-\frac{1}{2}R\right) + \frac{1}{2}\left(\exp\left(-i\int\limits_{-\infty}^{\infty} \varepsilon^s dt\right) - \right.$$
$$\left. - \exp\left(-i\int\limits_{-\infty}^{\infty} \varepsilon^a dt\right)\right) \varphi^Q_{n_0}\left(r+\frac{1}{2}R\right).$$

Первое слагаемое здесь соответствует обычному рассеянию, а второе - перезарядке. Квадрат модуля коэффициента при $\varphi^Q_{n_0}\left(p+\frac{1}{2}R\right)$ дает вероятность перезарядки

$$W(\rho) = \left|\sin\left(\frac{1}{2}\int\limits_{-\infty}^{\infty}\left(\varepsilon^a-\varepsilon^s\right)dt\right)\right|^2 = \left|\sin\left(\int\limits_{0}^{\infty}\left(\varepsilon^a-\varepsilon^s\right)dt\right)\right|^2,$$

где ρ - прицельный параметр.

Мы считаем, что величины $\varepsilon^a(R)$ и $\varepsilon^s(R)$ известны из рсшения задачи с неподвижными ядрами. Предполагая траекторию налетающей частицы прямолинейной, заменим интегрирование по t интегрированием по R. Так как $R^2 = \rho^2 + v^2t^2$, то

$$dt = \frac{1}{v}\frac{RdR}{\sqrt{R^2-\rho^2}}.$$

Обозначая $\varepsilon^a(R) - \varepsilon^s(R) \equiv \Phi(R)$, из (2.36) находим

$$W(\rho) = \left|\sin\left(\frac{1}{v}\int\limits_{i}^{\infty}\Phi(R)\frac{RdR}{\sqrt{R^2-\rho^2}}\right)\right|^2.$$

Рассмотрим прицельные расстояния $\rho \sim 1$. Тогда расстояния между частицами, существенные при взаимодействии, также порядка 1. Следовательно, весь интеграл в (2.37) порядка 1. Поскольку $v \ll 1$, то выражение для $W(\rho)$ сильно меняется при малом изменении ρ. Усредним (2.37) по некоторому интервалу значений ρ, малому по сравнению с ρ:

$$\bar{W} = \sqrt{\left|\sin\left(\frac{1}{v}\int\limits_{\rho}^{\infty}\Phi(R)\frac{RdR}{\sqrt{R^2-\rho^2}}\right)\right|^2} = \frac{1}{2},$$

т. е. перезарядка будет в половине всех случаев. Рассмотрим теперь вероятность перезарядки при $\rho \gg 1$. Как можно показать), при больших расстояниях между протонами разность энергий симметричного и антисимметричного состояний равна

$$\varepsilon^a(R) - \varepsilon^s(R) \underset{R\to\infty}{\approx} \frac{4}{e} R e^{-R}.$$

Поэтому при $\rho \gg 1$ получаем

$$\begin{aligned} F(\rho) &\equiv \frac{1}{v}\int\limits_0^\infty \Phi(R)\frac{RdR}{\sqrt{R^2-\rho^2}} = \frac{4}{ev}\int\limits_\rho^\infty \frac{R^2 e^{-R}}{\sqrt{R^2-\rho^2}}dR = \\ &= \frac{4\rho^2}{ev}\int\limits_1^\infty \frac{x^2 e^{-\rho x}}{\sqrt{x^2-1}}dx = \frac{4\rho^2 e^{-p}}{ev}\int\limits_0^\infty \frac{(z+1)^2 dz}{\sqrt{2(z+2)}} e^{-pz} \approx \\ &\approx \frac{4\rho^2}{ev} e^{-p}\frac{1}{\sqrt{2}}\int\limits_0^\infty z^{-1/2} e^{-\rho z} dz = \frac{4\rho^2}{ev} e^{-\rho}\frac{1}{\sqrt{2}}\frac{1}{\sqrt{\rho}}\Gamma\left(\frac{1}{2}\right) = \\ &= \frac{\pi\sqrt{2}}{ev}\rho^{3/2} e^{-\rho}. \end{aligned}$$

Мы видим, что $F(\rho) \ll 1$ при $\rho \gg \rho_1 \sim \ln 1/0$. Следовательно,

$$W = |\sin F(\rho)|^2 \approx F^2(\rho) = \frac{2\pi^2}{e^2 v^2}\rho^3 e^{-2\rho}.$$

Таким образом, при $\rho \ll \rho_1$ величина $F(\rho) \gg 1$, а при $\rho \geqslant \rho_1$ величина $F(\rho) \ll 1$.
Теперь оценим полное сечение перезарядки

$$\sigma = \int\limits_0^\infty \sin^2 F(\rho)\cdot 2\pi\rho d\rho.$$

По порядку величины получаем

$$\sigma = \int\limits_0^{\Gamma_1} \frac{1}{2} 2\pi\rho d\rho = \frac{1}{2}\pi_{\rho_1}^2 \sim \frac{1}{2}\pi \ln^2\frac{1}{v}.$$

Таким образом, при малых скоростях v ссчение перезарядки много болише геометрического сечения.

6.7.3 Berry's Phase: Basics

Appearance of Berry's Phase

При переходе под влиянием адиабатического изменения параметров гамильтониана в другие состояния экспоненциально редки, что следует из эволюции коэффициентов $c_{m\neq n}$. Теперь перейдём к обсуждению эволюции самого коэффициента c_n. При этом достаточно очевидно, что ничего кроме «накручивания» фазы с коэффициентом происходить не может. (???? why???)

Итак, уравнение $i\partial_t c_n(t) = -i\sum_m \exp\left(i\int_{t_0}^t \omega_{nm}(\tau)d\tau\right)\langle n(t)|\partial_t|m(t)\rangle c_m(t)$, с $m = n$ записывается и тривиально интегрируется:

$$\frac{dc_n(t)}{dt} = ic_n(t)\left\langle \psi_n(t)\left| i\frac{\partial}{\partial t}\right|\psi_n(t)\right\rangle$$

поэтому:

$$c_n(t) = c_n(0)\exp\left(i\gamma_n(t)\right),$$

где так называемая фаза Бери есть:

$$\gamma_n(t) := \int dt \cdot i \left\langle \psi_n(t) | \frac{\partial \psi_n(t)}{\partial t} \right\rangle$$

Свойства фазы Берри (???)

Исследуем полученный объект.

Фаза Берри действительно фаза.

Убедимся, что это действительно фаза - а именно, что эта величина вещественная.

Сделать это просто, дифференцируя условие нормировки мгновенных стационарных состояний:

$$0 = \partial_t \langle n(t)|n(t)\rangle = \left(\partial_t \langle n(t)|\right)|n(t)\rangle + \langle n(t)\,|\partial_t|\,n(t)\rangle = 2\,\mathrm{Re}\left(\langle n(t)\,|\partial_t|\,n(t)\rangle\right)$$

поэтому

$$\langle n(t)\,|i\partial_t|\,n(t)\rangle \in \mathbb{R}$$

Formula of a Berry's phase in terms of Berry's connection

Мы можем рассмотреть случай, когда гамильтониан зависит не явно от времени, но зависит от какого-то конечного набора параметров R_i : $\hat{H} = \hat{H}(\boldsymbol{R})$, которые, в свою очередь, как-то меняются со временем - описывают некоторую траекторию $\boldsymbol{R}(t)$ в пространстве параметров.

В свою очередь, мгновенные состояния гамильтониана тоже являются функциями этих параметров $|\psi_n\rangle = |\psi_n(\boldsymbol{R})\rangle$. Тогда выражение для фазы Берри можно переписать:

$$\gamma_n = \int dt \cdot i \,\langle \psi_n(\boldsymbol{R})|\nabla_{\boldsymbol{R}}\psi_n(\boldsymbol{R})\rangle \cdot \frac{\partial \boldsymbol{R}}{\partial t} = \int \boldsymbol{A}_n(\boldsymbol{R}) d\boldsymbol{R}, \quad \boldsymbol{A}_n(\boldsymbol{R}) = i\,\langle \psi_n(\boldsymbol{R})|\nabla_{\boldsymbol{R}}\psi_n(\boldsymbol{R})\rangle$$

Это - криволинейный интеграл.

Величина $\boldsymbol{A}(\boldsymbol{R})$ носит название связности Берри и является вектором, живущем в томже пространстве параметров.

В такой записи видно следующее немаловажное свойство: фаза Берри не зависит от того, *как* именно мы меняем параметры $\boldsymbol{R}(t)$ (лишь бы это было адиабатически) - но зависит только от вида самой траектории в пространстве параметров.

Из-за этого фундаментального свойства фазу Берри называют также геометрической фазой.

Berry's phase is not gauge invariant

Связность и фаза Берри не являются калибровочно-инвариантными величинами.

Априори выбор фазы собственных состояний $|\psi_n(R)\rangle$ произволен - мы лишь требуем, чтобы оно было собственным для гамильтониана $\hat{H}(\boldsymbol{R})$. Вместо набора состояний можно выбрать любой другой $-\left|\widetilde{\psi}_n(\boldsymbol{R})\right\rangle = e^{i\chi(\boldsymbol{R})}\,|\psi_n(\boldsymbol{R})\rangle$ (это называется калибровочным преобразованием); формулы для связности и фазы изменятся:

$$\widetilde{\boldsymbol{A}}_n(\boldsymbol{R}) = \boldsymbol{A}_n(\boldsymbol{R}) - \nabla\chi, \quad \widetilde{\gamma}_n = \gamma_n - \chi\left(\boldsymbol{R}_f\right) + \chi\left(\boldsymbol{R}_i\right)$$

Where is the meaning of Berry's phase?

(????? don't know)

Is Berry's phase really important?

(????? don't know. I don't see why it is important, but there are many books that deal with it. But this is the minority, anyway)

Applications in topological materials (???)

(???? there are thousands articles about it, I'll write an overview here)

Where does Berry's phase is also used?

(??? write answer to it, currently, i don't know. And how exactly??)

О применениях во вращающихся спиновых системах в магнитном поле (??)

(???)

О применениях в эффекте Холла (???)

(??? как догадаться, что эффект Холла может быть объяснен с ней?)
(На ютубе хорошо объяснено.)

Experimental confirmation of Berry's phase

This was the first experiment to confirm the prediction of Berry. It was purposed by R.Y. Chiao and Y.S. Wu [10] in 1986 and this year yet realized by A. Tomita and R.Y. Chiao [6]. The photon's spin vector, which points either along the direction in which it is traveling or in the opposite direction, can be easily turned by changing the direction of travel. In [10] and [6], it is done with a coiled optical fibre.

[6] A. Tomita, R. Y. Chiao, "Observation of Berry's topological phase by use of an optical fibre", Phys. Rev. Lett. 57 (1986) 937-940.

[10] R.Y. Chiao and Y.S. Wu, "Manifestations of Bery's topological phase for the photon", Phys. Rev. Lett. 57 (1986) 933-936.

(this is really interesting, but no time for it now)

Спин в магнитном поле как пример адиабатических методов

Классическая задача, иллюстрирующая фазу Берри - задача о движении спина $\frac{1}{2}$ в медленно меняющемся магнитном поле.

Гамильтониан системы имеет следующий вид:

$$\hat{H}(\boldsymbol{B}) = -\boldsymbol{B} \cdot \hat{\boldsymbol{\sigma}}$$

где $\hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ -матрицы Паули.

Основное состояние системы соответствует спину, поляризованному вдоль поля.

Если теперь поле заставить пройти замкнутый цикл (при этом наш спин адиабатически будет следить за полем, в силу адиабатической теоремы), то в конце мы получим исходное состояние.

Изучим, как устроена фаза Берри для данной задачи.

Изучать её мы будем в сферических координатах: $B = (B\sin\theta\cos\varphi, B\sin\theta\sin\varphi, B\cos\theta)$. Сперва нам требуется найти мгновенные собственные состояния гамильтониана:

$$\hat{H} = -B\begin{pmatrix} \cos\theta & \sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & -\cos\theta \end{pmatrix}, \quad \begin{cases} E_+ = +B, & |\psi_+\rangle = \begin{pmatrix} \sin\frac{\theta}{2} \\ -e^{i\varphi}\cos\frac{\theta}{2} \end{pmatrix} \\ E_- = -B, & |\psi_-\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\varphi}\sin\frac{\theta}{2} \end{pmatrix} \end{cases}$$

Ключевых параметра тут 2 -углы θ и φ (имеются в виду параметры, задающие вектор R; изменение длины B, как мы видим, на волновые функции не влияет никак).

Поэтому у связности Берри будет две компоненты:

$$A_\theta^{(-)} = i\left\langle \psi_- | \frac{\partial\psi_-}{\partial\theta} \right\rangle = 0, \quad A_\varphi^{(-)} = i\left\langle \psi_- | \frac{\partial\psi_-}{\partial\varphi} \right\rangle = -\sin^2\frac{\theta}{2} = -\frac{1}{2}(1-\cos\theta)$$

и поэтому для любой замкнутой эволюции фаза Берри будет иметь вид:

$$\gamma_- = -\frac{1}{2}\oint(1-\cos\theta)d\varphi = -\frac{1}{2}\Omega$$

В действительности же, этот интеграл в точности равен телесному углу, который заметает замкнутая траектория на единичной сфере.

Проще всего это продемонстрировать в простом случае $\theta = \text{const} \to \gamma = -\pi(1-\cos\theta)$; в то время как телесный угол равен $2\pi(1-\cos\theta)$. Это - демонстрация того факта, что фаза Берри является геометрической фазой, в данной задаче она определяется чисто геометрической характеристикой траектории.

Сделаем ещё несколько замечаний: Телесный угол ориентирован - если изменить направление обхода контура, то поменяется и знак Ω.

Можно выбрать как телесный угол «внутри» контура Ω, так и телесный угол «вне» контура, $4\pi-(-\Omega)$ -при этом знак Ω поменяется из-за неправильного направления обхода.

Очевидно, что полученные фазы Берри отличаются на 2π -что не является большой проблемой, ведь это фаза.

Этот результат достаточно просто обобщается на произвольный спин S (не $\frac{1}{2}$) и на состояние с произвольной проекцией $M \in [-S, S]$ на направление магнитного поля - ответ записывается как $\gamma_M = M\Omega$. Поскольку M бывает либо полуцелым, либо цельм, то проблем с неоднозначностью фазы не возникает:

утверждение про калибровочную неинвариантность связаности Берри можно тут продемонстрировать явно.

Действительно, можно выбрать волновую функцию, скажем, в чуть ином виде: $\left|\widetilde{\psi}_-\right\rangle = \begin{pmatrix} e^{-i\varphi}\cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}$.

Это изменит и выражение для связности Берри, $\widetilde{A}_\varphi^{(-)} = \frac{1}{2}(1+\cos\theta)$. Однако выражение для интеграла от фазы по замкнутому контиуру при этом не изменится (разумеется, по модулю 2π).

Наконец, отметим, что в современной физике конденсированного состояния к фазе Берри проявляется огромный интерес, связанный с её применениями при исследовании топологических изоляторов.

В них фаза Берри играет ключевую роль, и именно в связи с ней эти вещества проявляются нетривиальные (топологические) свойства.

6.7.4 Extra Understanding of Geometrical Phases 1

(this theory is for applications and for connection with condensed matter, I'll later write it better, since topology is popular in condensed matter)

Introduction by Michael El-Batanouny

Known derivation in another formalism

In this chapter, we need to develop the formalism of Berry's geometric quantum phase. It is a manifestation of cyclic, adiabatic time evolution of Hamiltonians $\mathcal{H}[\eta(t)]$ controlled by a time-dependent, multidimensional parameter $\eta(t)$. For example, the parameter may determine variations in external magnetic and electric fields, or ionic coordinates in the Born-Oppenheimer approximation. It could also be, as we will need later, the crystal momentum $\mathbf{k}$ in a Brillouin zone. In general, η is defined on an n-dimensional parameter space $\eta(t) \equiv \{\eta_1(t), \eta_2(t), ..., \eta_n(t)\}$.$\mathcal{H}(\eta)$ and its energy spectrum $\varepsilon_\mu(\eta)$ depend smoothly on the parameter η.

For simplicity, we consider a quantum-mechanical system with a discrete and nondegenerate energy spectrum, with the proviso that no energy level crossing occurs during time evolution. As we have learned, for such systems the adiabatic theorem in quantum mechanics surmises that for a slowly changing Hamiltonian, the system remains in its evolving, time-dependent ground- or eigen-state. But, as revealed by Michael Berry in 1983, this is actually very incomplete [27, 159]. To understand the rationale behind this assertion, we consider the slow time variation of a Hamiltonian through its dependence on a parameter $\eta(t)$. We seek solutions for the Schrödinger equation

$$i\frac{\partial\psi(t)}{\partial t} = \mathcal{H}[\eta(t)]\psi(t), \quad \psi(t) \in \mathbb{H}$$

For adiabatic time evolution, we write the general solution of the Schrödinger equation as

$$\psi(t) = \sum_\mu c_\mu(t)|\mu, \eta(t)\rangle.$$

Substituting in (10.1), we get the following equation for the coefficients

$$\dot{c}_\mu(t) = -i\varepsilon_\mu(t)c_\mu(t) - \sum_v c_v(t)\left\langle \mu, \eta(t)\left|\partial_t\right|v, \eta(t)\right\rangle .$$

Thus, if we start with a certain $c_\mu(0) = 1, c_\nu(0) = 0, \forall\nu \neq \mu$, the adiabatic assumption is approximately fulfilled when $\langle \mu, \boldsymbol{\eta}(t)\left|\partial_t\right| v, \boldsymbol{\eta}(t)\rangle$ are small for $v \neq \mu$. We can show, by substituting in the eigenvalue equation

$$\mathcal{H}(t)|v, \boldsymbol{\eta}(t)\rangle = \varepsilon_v(t)|v, \boldsymbol{\eta}(t)\rangle,$$

that this matrix element can be expressed as

$$\left\langle \mu, \boldsymbol{\eta}(t)\left|\partial_t\right| v, \boldsymbol{\eta}(t)\right\rangle = \frac{\left\langle \mu, \boldsymbol{\eta}(t)\left|\partial_t\mathcal{H}(t)\right| v, \boldsymbol{\eta}(t)\right\rangle}{\varepsilon_v(t) - \varepsilon_\mu(t)} \ll 1 \quad \text{adiabatic assumption.}$$

Under the adiabatic assumption, we can directly solve (10.3) for $c_\mu(t)$ by integration, and obtain

$$\begin{aligned}
c_\mu(t) &= e^{-i\int_0^t d\tau \varepsilon_\mu(\tau)} e^{i\int_0^t d\tau i\langle \mu,\eta(\tau)|\partial_\tau|\mu,\eta(\tau)\rangle} = e^{i\alpha_{\rm dyn}(t)} e^{i\gamma(t)} \\
\psi(t) &= e^{i\alpha_{\rm dyn}(t)} e^{i\gamma(t)} |\mu,\eta(t)\rangle \\
\gamma &= \int_0^t d\tau i \left\langle \mu,\eta(\tau)\right| \left|\partial_\tau\right| \mu,\eta(\tau)\rangle = \int_0^t d\tau i \left\langle \mu,\eta(\tau)\right| \left|\nabla_\eta\right| \mu,\eta(\tau)\rangle \cdot \frac{d\eta}{d\tau} \\
&= \int_{\eta(0)}^{\eta(t)} i \left\langle \mu,\eta\right| \left|\nabla_\eta\right| \mu,\eta\rangle \cdot d\eta.
\end{aligned}$$

where the phase α arises from the usual dynamics, but γ is a manifestation of geometric aspects of the system evolution.

What Michael Berry demonstrated was that when the Hamiltonian evolves adiabatically around a closed loop C in η-space, with $n > 1$, an irreducible geometric phase γ relative to the initial state may emerge, namely, γ was coined Berry's phase by Barry Simon in 1983 [167], where he revealed the intimate connection between Berry's phase and holonomy on a line bundle.

10.1.1 Berry's Vector Potential, Field, and Flux

We find that the formulation becomes very easy to visualize when η is a three-dimensional parameler where ordinary vector calculus can be invoked. Here, we say that for a nondegenerate state, the only freedom in the choice of reference functions is a local phase

$$\psi(\eta) \to e^{i\theta(\eta)}\psi(\eta).$$

Under this modification, $\mathcal{A}$ in (10.6) changes by a gradient

$$\mathcal{A} \to \mathcal{A} + \nabla_\eta \theta,$$

a gauge transformation reminiscent of the vector potential in electrodynamics, and $\mathcal{A}$ is sometimes referred to as Berry's vector potential. So the integrals of $\mathcal{A}$ around closed loops C

$$\oint_C \mathcal{A} \cdot d\boldsymbol{\ell}_\eta$$

will be gauge invariant. We can use Stokes, theorem and write

$$\gamma = \oint_C \mathcal{A} \cdot d\eta \mod 2\pi = \iint_{S(C)} \mathcal{F} \cdot d\mathbf{S}_\eta \bmod 2\pi,$$

where $d\mathbf{S}_\eta$ denotes the area element in η space, and the integral is performed over any surface bounded by the closed contour C. Again, by analogy with electrodynamics, $\mathcal{F}$ is sometimes called the Berry field, and is defined as

$$\begin{aligned}
\mathcal{F} &= \nabla_\eta \times \mathcal{A} \\
\mathcal{F}_{\alpha\beta} &= \partial_\alpha \mathcal{A}_\beta - \partial_\beta \mathcal{A}_\alpha = -2\mathrm{Im}\left\langle \partial_\alpha \psi(\eta) | \partial_\beta \psi(\eta)\right\rangle.
\end{aligned}$$

Thus, this mathematical structure has evoked analogies with classical electromagnetism. We can envision $\mathcal{A}$ as abstract vector potential in parameter space, and $\mathcal{F}$ as a magnetic field.

Following this analogy, we surmise from (10.8) that Berry's phase γ is akin to a flux through the surface $\mathbf{S}$. We recall that a vector potential has considerable gauge arbitrariness, and has no physical meaning, while its loop integral is indeed gauge invariant and observable.

The set of phase factors $e^{i\theta(\eta)}$ form the group $U(1)$ of unitary 1×1 matrices. We therefore have a gauge theory with gauge (symmetry) group $U(1)$ and gauge potential $\mathbf{A}(\eta)$

The loop integral of the Berry potential, the Berry phase γ, is nontrivial in two cases:

- Curl $\mathcal{A}$ is nonzero.
- The curl is zero but the curve C is not in a simply connected domain.

We can invoke a generalized Stokes' theorem in any dimension of η parameter space, when C is the boundary of a surface $\mathbf{S}(C)$ in a simply connected domain, and the curl of $\mathcal{A}$ is regular on $\mathbf{S}(\mathcal{C})$.

$\mathcal{A}$ as a Berry Connection by Michael El-Batanouny

Now, we shall recast $\mathcal{A}$ as a topological geometric structure. We first note that the unitarity of time evolution preserves the scalar product, allowing the family of Hamiltonians $\mathcal{H}(\boldsymbol{\eta})$ to share the Hilbert space HI, and normalized state vectors to remain normalized and confined to the sphere $\mathbb{S}^{2\mathcal{N}+1}$. Consequently, the projected physical-state manifold $\mathbb{P}(\mathbb{H})$ continues to be the base manifold of the principal line bundle $\mathbb{E}$, with the fiber $\mathbb{F}$ being the unitary group $U(1)$.$\mathbb{P}(\mathbb{H})$ is homeomorphic with η.

We still focus on the spectrum of discrete, isolated, and nondegenerate eigenvalues $\varepsilon_\mu(\eta)$ with corresponding normalized eigenkets $\psi_\mu(\eta)$.[1] We recall that the set of equivalent normalized eigenkets $e^{i\phi}\psi(\eta) = \psi(\phi, \eta)$ form a ray, and share the projection $\pi = |\psi(\eta)\rangle\langle\psi(\eta)| \in \mathbb{P}(\mathbb{H})$. The adiabatic time dependence of $\mathcal{H}$ amounts to traversing a curve $t \to \eta(t)$ in η at adiabatically slow velocity. We also note that a cyclic evolution, $\eta(0) = \eta(T)$, is uniquely associated with a loop $\mathcal{C}(\eta)$ in η, or in $\mathbb{P}(\mathbb{H})$.

From another perspective, we can envision that time evolution produces a path in the total space $\mathbb{E}$. The corresponding path in the space of physical states $\mathbb{P}(\mathbb{H}) \simeq \eta$ is obtained by a π projection of the path in $\mathbb{E}$ onto the base manifold. In the cyclic evolutions we are interested in, we find that the system terminates in the initial physical state, and the paths are represented by closed curves in η. Closed paths in η may correspond to closed or open paths in $\mathbb{E}$. In a cyclic evolution, an open path in $\mathbb{E}$ means that a state vector terminates on the same initial fiber, but it lands on another state vector that differs from the initial state vector by an overall phase.

$U(1)$ A Transition Functions and Gauge Transformations

We note that, in general, each wavefunction $\psi(\eta)$ can be chosen to be smooth only over patches of η, but not necessarily over the whole of η. In other words, the set of state vectors $\psi(\phi, \eta)$ form a smooth section over each patch $\mathbb{U} \subset \eta$. For two overlapping patches $\mathbb{U}_1 \cap \mathbb{U}_2 \neq \emptyset$, with sets of smooth functions $\psi^{(1)}(\eta)$ and $\psi^{(2)}(\eta)$, respectively, we know that for any $\eta \in \mathbb{U}_1 \cap \mathbb{U}_2$ the corresponding functions share the same ray above η, and can differ only by a complex phase, $\theta(\boldsymbol{\eta}), e^{i\theta(\eta)} \in U(1)$, namely,

$$\psi^{(2)}(\eta) = e^{i\theta(\eta)}\psi^{(1)}(\eta),$$

which is just a gauge transformation. Both $\psi^{(1)}(\eta)$ and $\psi^{(2)}(\eta)$ constitute a possible set of instantaneous solutions, and the freedom in choice of either one or another manifests the gauge freedom. The corresponding group that is used to formulate the condition of the gauge freedom is called the gauge group. In our case, the gauge group is $U(1)$.

10.2.1 Construction of the Berry Connection

Before constructing the connection [34], which is associated with the horizontal subspace, we shall identify the vertical subspace, or the vertical direction. We recall that the fibers are generated by the action of the group $U(1)$ on the physical states of the base manifold $\mathbb{P}(\boldsymbol{\eta})$

$$\psi(\phi, \boldsymbol{\eta}) = e^{i\phi}\psi(\boldsymbol{\eta}), \quad \psi(\boldsymbol{\eta}) \in \mathbb{P}(\boldsymbol{\eta})$$

This means that the normalized states of a fiber differ by a phase from each other, and, thus, point in the same direction - the vertical direction generated by the $U(1)$ action.

Since the line bundle is embedded in a complex vector space, a natural way to construct the connection (a horizontal subspace) is to use the corresponding metric, the scalar product. We can decompose the tangent vectors

$$\frac{d\psi(\phi(t), \boldsymbol{\eta}(t))}{dt} = \partial_t \psi(\phi(t), \boldsymbol{\eta}(t)) \in TE$$

to the curve $\psi(\phi(t), \eta(t)) \in \mathbb{E}$, with the aid of the scalar product, into vertical and horizontal components, as

$$\begin{aligned} \frac{d\psi(\phi(t), \eta(t))}{dt} &= \langle \psi(\phi(t), \eta(t)) | \partial_t \psi(\phi(t), \eta(t)) \rangle \, |\psi(\phi(t), \eta(t))\rangle \\ &\quad + |h_\psi(t)\rangle \text{ (horizontal component)} \\ \langle \psi(\phi(t), \eta(t)) | h_\psi(t) \rangle &= 0, \quad \text{parallel transport} \end{aligned}$$

To evaluate the connection explicitly, we need to consider a local patch $\mathbb{U} \subset \eta$ and the region of $\mathbb{E}$ over $\mathbb{U}$. Since tangent vectors in TE are produced by the operator d/dt, we split it into vertical and horizontal operators as

$$\frac{d}{dt} = a_v \frac{\partial}{\partial \phi} + \sum_\alpha b_h^\alpha D_\alpha = a_v \frac{\partial}{\partial \phi} + \sum_\alpha b_h^\alpha \left[\frac{\partial}{\partial \eta^\alpha} + \mathcal{A}_\alpha \frac{\partial}{\partial \phi} \right],$$

where the first term corresponds to the vertical subspace, since it clearly depends only on variations in the phase ϕ. We therefore write

$$\begin{aligned} \langle \psi(\phi(t), \boldsymbol{\eta}(t)) | \partial_t \psi(\phi(t), \boldsymbol{\eta}(t)) \rangle \, |\psi(\phi(t), \boldsymbol{\eta}(t))\rangle &= a_v \frac{\partial}{\partial \phi} |\psi(\phi(t), \boldsymbol{\eta}(t))\rangle \\ |h_\psi\rangle = \sum_\alpha b_h^\alpha D_\alpha |\psi(\phi(t), \boldsymbol{\eta}(t))\rangle & \end{aligned}$$

and, according to (10.11), we obtain

$$\langle \psi(\phi(t), \eta(t)) \, | b_h^\alpha D_\alpha | \, \psi(\phi(t), \boldsymbol{\eta}(t)) \rangle = 0.$$

Since b_h^α is arbitrary, we find that

$$\left\langle \psi(\phi(t), \boldsymbol{\eta}(t)) \left| \frac{\partial}{\partial \eta^\alpha} + \mathcal{A}_\alpha \frac{\partial}{\partial \phi} \right| \psi(\phi(t), \boldsymbol{\eta}(t)) \right\rangle = 0.$$

Using the fact that $|\psi(\phi(t), \eta(t))\rangle$ is normalized, and that

$$\frac{\partial}{\partial \phi} |\psi(\phi(t), \boldsymbol{\eta}(t))\rangle = \frac{\partial}{\partial \phi} e^{i\phi} \psi(\eta) = i |\psi(\phi(t), \eta(t))\rangle,$$

we obtain

$$\mathcal{A}_\alpha \left\langle \psi(\phi(t),\boldsymbol{\eta}(t)) \left| \frac{\partial}{\partial \phi} \right| \psi(\phi(t),\boldsymbol{\eta}(t)) \right\rangle = i\mathcal{A}_\alpha \langle \psi(\phi(t),\boldsymbol{\eta}(t)) | \psi(\phi(t),\boldsymbol{\eta}(t)) \rangle$$
$$= - \left\langle \psi(\phi(t),\boldsymbol{\eta}(t)) \left| \frac{\partial}{\partial \eta^\alpha} \right| \psi(\phi(t),\boldsymbol{\eta}(t)) \right\rangle$$

or

$$\mathcal{A}_\alpha = i \left\langle \psi(\phi(t),\boldsymbol{\eta}(t)) \left| \frac{\partial}{\partial \eta^\alpha} \right| \psi(\phi(t),\boldsymbol{\eta}(t)) \right\rangle .$$

The connection $\mathcal{A}$ is then given by the one-form

$$\mathcal{A} = \sum \mathcal{A}_\alpha d\eta^\alpha = i\langle \psi(\phi(t),\eta(t)) | d | \psi(\phi(t),\eta(t)) \rangle$$

defined on the line bundle in terms of the covariant derivative $\nabla_{\boldsymbol{\eta}}$. Thus, $\mathcal{A}$ is also referred to as the Berry connection. [2]

The horizontal lift

With the construction of the connection in hand, we proceed to define the horizontal lift. The horizontal lift involves lifting the tangent vectors to the curve in η up along the fibers and orienting them such that they are horizontal. Consequently, for $|\psi(\phi,\eta)\rangle$ to be a horizontal lift, the vertical part of $|\partial_t \psi(\phi,\eta)\rangle$ must vanish

$$\langle \psi(\phi,\eta) | \partial_t \psi(\phi,\eta) \rangle = 0.$$

This condition is called the horizontal lift equation or the equation for parallel transport. We have invoked the notion of parallel transport in the line bundle $\mathbb{E}$ in a manner completely analogous to the way an ordinary covariant derivative on a smooth manifold defines parallel transport in the tangent bundle of the smooth base. As we will show, the twisting of this line bundle affects the phase of quantum mechanical wave functions.

In bundle language, $|\psi(\phi,\eta)\rangle$ can be considered as a local section of the fiber bundle, namely, a continuous mapping of a patch $\mathbb{U} \subset \eta$ into the fibers above $\mathbb{U}$. A change to a different patch $\mathbb{U}' \subset \eta$ corresponds to a change in the section

$$|\psi(\phi(\boldsymbol{\eta}),\boldsymbol{\eta})\rangle \to |\psi\left(\phi'(\boldsymbol{\eta}),\boldsymbol{\eta}\right)\rangle$$
$$|\psi\left(\phi'(\boldsymbol{\eta}),\boldsymbol{\eta}\right)\rangle = e^{i\theta(\eta)} |\psi(\phi,\eta)\rangle$$

This means that the connection transforms as

$$\mathcal{A}'_\alpha = \mathcal{A}_\alpha - \frac{\partial \theta(\eta)}{\partial \eta^\alpha},$$

a gauge transformation. We note that a local section, being a section over a single patch, maps a closed path in η, with $\eta(T) = \eta(0), 0 \le t \le T$, into a closed path in $\mathbb{E}$. We will denote the closed path in $\mathbb{E}$ as $|\psi(\eta(t))\rangle$, with $|\psi(\eta(T))\rangle = |\psi(\eta(0))\rangle$. A gauge transformation gives a different closed path in $\mathbb{E}$,

$$|\psi_\theta(\eta(t))\rangle = e^{i\theta(t)} |\psi(\eta(t))\rangle.$$

In order for $|\psi_\theta(\eta(t))\rangle$ to be closed, the function θ must satisfy

$$\theta(T) = \theta(0) + 2n\pi$$

with n integer.

10.2.2 Holonomy and Berry's Phase

We will now evaluate the holonomy produced by the horizontal lift of a closed curve in η with respect to the connection we previously derived (see Figure 10.1). We denote the horizontal lift by $|\psi_h(\eta(t))\rangle$. By definition, the tangent vectors to the curve $|\psi_h(\eta(t))\rangle$ must be horizontal. According to (10.10), this means

$$\langle\psi_h(\phi,\eta)|\partial_t\psi_h(\eta(t))\rangle = 0.$$

We can express the open path $|\psi_h(\boldsymbol{\eta}(t))\rangle$ in $\mathbb{E}$ in terms of a closed path $|\psi(\phi(t),\boldsymbol{\eta}(t))\rangle$ in $\mathbb{E}$ as

$$\begin{aligned}
|\psi_h(\eta(t))\rangle &= e^{i\xi(t)}|\psi(\phi(t),\eta(t))\rangle \\
|\psi(\phi(T),\eta(T))\rangle &= |\psi(\phi(0),\eta(0))\rangle, \quad \phi(T) = \phi(0) + 2n\pi \\
|\psi_h(\eta(T))\rangle &= e^{i[\xi(T)-\xi(0)]}\,|\psi_h(\eta(0))\rangle\,.
\end{aligned}$$

Setting $\gamma = \xi(T) - \xi(0)$, substituting (10.17) into (10.16) and integrating, we obtain

$$\begin{aligned}
\langle\psi_h(\phi,\eta)|\partial_t\psi_h(\eta(t))\rangle =& i\xi(t)\langle\psi(\phi(t),\eta(t))|\psi(\phi(t),\eta(t))\rangle \\
&+ \langle\psi(\phi(t),\eta(t))|\psi(\phi(t),\eta(t))\rangle \\
\xi(t) =& i\langle\psi(\phi(t),\eta(t))|\psi(\phi(t),\eta(t))\rangle \\
\gamma =& i\int_0^T dt\,\langle\psi(\phi,\eta(t))|\partial_t\psi(\phi,\eta(t))\rangle
\end{aligned}$$

The tangent vector $|\dot{\psi}(\phi(t),\eta(t))\rangle$ is given by

$$\frac{d}{dt}|\psi(\phi(t),\boldsymbol{\eta}(t))\rangle = \dot{\phi}\frac{\partial|\psi(\phi(t),\eta(t))\rangle}{\partial\phi} + \sum_\alpha \dot{\eta}^\alpha \frac{\partial|\psi(\phi,\boldsymbol{\eta}(t))\rangle}{\partial\eta^\alpha}$$

and we write

$$\begin{aligned}
\gamma =& i\int_0^T dt\dot{\phi}\left\langle\psi(\phi,\eta(t))\left|\frac{\partial}{\partial\phi}\right|\psi(\phi,\eta(t))\right\rangle \\
&+ i\int_0^T dt\eta^\mu\left\langle\psi(\phi,\eta(t))\left|\frac{\partial}{\partial\eta^\mu}\right|\psi(\phi,\eta(t))\right\rangle \\
=& -\int_{\phi(0)}^{\phi(T)} d\phi + i\int_{\eta^\mu(0)}^{\eta^\mu(T)} d\eta^\mu\left\langle\psi(\eta)\left|\frac{\partial}{\partial\eta^\mu}\right|\psi(\eta)\right\rangle \\
=& -2n\pi + \oint_{\mathcal{C}}\langle\psi(\eta)|d|\psi(\eta)\rangle = -2n\pi + \oint_{\mathcal{C}}\mathcal{A} = \gamma(\mathcal{C}),
\end{aligned}$$

where $\mathcal{C}$ is the closed path in $\eta\cdot\langle\psi(\eta)|d|\psi(\eta)\rangle$ is purely imaginary, since for normalized states $|\psi(\eta)\rangle$

$$\begin{aligned}
\frac{\partial}{\partial\eta^\mu}\langle\psi(\eta)|\psi(\eta)\rangle = 0 &= \left\langle\psi(\eta)|\frac{\partial}{\partial\eta^\mu}\psi(\eta)\right\rangle + \left\langle\frac{\partial}{\partial\eta^\mu}\psi(\eta)|\psi(\eta)\right\rangle \\
&= 2\,\mathrm{Re}\left\langle\psi(\eta)|\frac{\partial}{\partial\eta^\mu}\psi(\eta)\right\rangle
\end{aligned}$$

10.2.3 The Berry Curvature

If the base η is simply connected, then expression (10.18) for the Berry phase can be rewritten as a surface integral of the local curvature form. Using Stokes' theorem, we write

$$\gamma(\mathcal{C}) = \int\limits_{S(\mathcal{C})} \mathcal{F} \cdot d\mathbf{S},$$

where $S(\mathcal{C})$ is an arbitrary submanifold, of dimension $n-1$, bounded by $\mathcal{C}$, namely, $\delta\mathbf{S} = \mathcal{C}$, and

$$\mathcal{F} = d\mathcal{A} = -\eta\langle d\psi(\eta)|d\psi(\eta)\rangle \quad \text{two-form}$$

is the Berry curvature. In local coordinates on η it is given by the two-form

$$\begin{aligned}\mathcal{F} &= \frac{1}{2}\mathcal{F}_{ij} d\eta_i \wedge d\eta_j \\ \mathcal{F}_{ij} &= -\mathrm{Im}\left(\langle\partial_i\psi|\partial_j\psi\rangle - \langle\partial_j\psi|\partial_i\psi\rangle\right).\end{aligned}$$

If the base η is not simply connected, then the expression for the Berry phase as surface integral (10.19) is valid only for those curves that are contractible to a point. Berry's Curvature in Terms of Hamiltonian Derivatives: Hidden Physics With

$$\mathcal{F}_n(\eta) = -\mathrm{Im}\,\langle d\psi_n(\eta)|d\psi_n(\eta)\rangle$$

we insert the identity operator, $\mathbb{I} = \sum_m |\psi_m\rangle\langle\psi_m|$, and we obtain

$$\begin{aligned}\mathcal{F}_n(\boldsymbol{\eta}) &= -\mathbf{3}\sum_m \langle d\psi_n(\boldsymbol{\eta})|\psi_m(\eta)\rangle \wedge \langle\psi_m(\boldsymbol{\eta})|d\psi_n(\eta)\rangle \\ &= -3\sum_{m\neq n} \langle d\psi_n(\boldsymbol{\eta})|\psi_m(\eta)\rangle \wedge \langle\psi_m(\eta)|d\psi_n(\eta)\rangle\end{aligned}$$

where the sum excludes $m = n$ since $\langle\psi_n(\eta)|d\psi_n(\eta)\rangle$ is purely imaginary. An important consequence of (10.22) is that the sum of Berry curvatures of all the eigenstates of the Hamiltonian is zero. If we consider Hamiltonians with discrete spectra along a closed path C, and sum over Berry's phases of all eigenstates, we obtain

$$\sum_n \mathcal{F}_n(\eta) = 0,$$

which follows from (10.22), since

$$\begin{aligned}\mathcal{F}_n^{ij}(\eta) &= -\,\mathrm{Im}\sum_{m\neq n}\left(\langle\partial_i\psi_n(\eta)|\psi_m(\eta)\rangle\langle\psi_m(\eta)|\partial_j\psi_n(\eta)\rangle - (i \rightleftharpoons j)\right) \\ &= -\frac{1}{2}\mathrm{Im}\sum_{m\neq n}\left(\langle\partial_i\psi_n(\eta)|\psi_m(\eta)\rangle\langle\psi_m(\eta)|\partial_j\psi_n(\eta)\rangle\right. \\ &\quad \left. + \langle\partial_j\psi_m(\eta)|\psi_n(\eta)\rangle\langle\psi_n(\eta)|\partial_i\psi_m(\eta)\rangle - (i \rightleftharpoons j)\right)\end{aligned}$$

since $\langle\partial_i\psi_n(\eta)|\psi_m(\eta)\rangle = -\langle\psi_n(\eta)|\partial_i\psi_m(\eta)\rangle$. It is clear then that

$$\sum_n \mathcal{F}_n^{ij}(\eta) = 0$$

since the sum is both symmetric and antisymmetric in i and j. Applying the exterior derivative d to the eigenvalue equation

$$\mathcal{H}(\boldsymbol{\eta})\,|\psi_n(\boldsymbol{\eta})\rangle = E_n(\boldsymbol{\eta})\,|\psi_n(\boldsymbol{\eta})\rangle$$

yields

$$d\mathcal{H}(\boldsymbol{\eta})\,|\psi_n(\boldsymbol{\eta})\rangle + \mathcal{H}(\boldsymbol{\eta})d\,|\psi_n(\eta)\rangle = dE_n(\boldsymbol{\eta})\,|\psi_n(\boldsymbol{\eta})\rangle + E_n(\boldsymbol{\eta})d\,|\psi_n(\boldsymbol{\eta})\rangle$$

and projecting onto $\langle\psi_m(\eta)|$, we get

$$\langle\psi_m(\eta)|d\mathcal{H}(\boldsymbol{\eta})|\psi_n(\eta)\rangle = (E_n(\eta) - E_m(\eta))\,\langle\psi_m(\eta)|d\psi_n(\eta)\rangle$$

or

$$\langle\psi_m(\eta)|d\psi_n(\eta)\rangle = \frac{\langle\psi_m(\eta)|d\mathcal{H}(\eta)|\psi_n(\eta)\rangle}{E_n(\eta) - E_m(\eta)}, \quad m \neq n$$

and

$$\mathcal{F}_n(\eta) = -\ni \sum_{m\neq n} \frac{\langle\psi_n(\eta)|d\mathcal{H}(\eta)|\psi_m(\eta)\rangle \wedge \langle\psi_m(\eta)|d\mathcal{H}(\eta)|\psi_n(\eta)\rangle}{(E_n(\eta) - E_m(\eta))^2}$$

We note that $\mathcal{F}_n$ becomes infinite at some $\eta - \eta^*$, if $E_n(\eta^*) - E_m(\eta^*)$, a δ-function like singularity that heralds the presence of a fictitious field source. We discern that the source is static; for example, it may manifest the nature of a magnetic monopole rather than currents.

We can surmise that wherever the ground state is degenerate, the curvature becomes ill defined and singular. In such a situation, the vicinity of the singularity must be excluded, which leads to a domain that is not simply connected.

Finally, (10.24) has the advantage that it is free of wavefunction differentiation, therefore it can be evaluated under any gauge choice. This property is particularly useful for numerical calculations, in which the condition of a smooth phase choice of the eigenstates is not guaranteed in standard diagonalization procedures. Isolated Degeneracies and Diabolical Points We consider a quantum system parameterized by $\eta = \{\eta_1, ..., \eta_n)$, and assume that for some point η^* two energy eigenvectors $\psi_1(\eta^*)$ and $\psi_2(\eta^*)$ are degenerate, with energy $E^* = E(\eta^*)$. Near the degeneracy point η^*, we may approximate the system as a two-level one, and write its Hamiltonian as

$$\mathcal{H} = \begin{pmatrix} \mathcal{H}_{11}(\eta) & \mathcal{H}_{12}(\eta) \\ \mathcal{H}_{12}^*(\eta) & \mathcal{H}_{22}(\eta) \end{pmatrix}$$

with eigenvalues

$$E_\pm = \frac{\mathcal{H}_{11} + \mathcal{H}_{22}}{2} \pm \sqrt{\left(\frac{\mathcal{H}_{11} - \mathcal{H}_{22}}{2}\right)^2 + |\mathcal{H}_{12}|^2}\,.$$

$$(\mathcal{H}_{11} - \mathcal{H}_{22})^2 + 4\,|\mathcal{H}_{12}|^2 = 0, \quad \mathcal{H}_{11} = \mathcal{H}_{22}, \quad \mathrm{Re}\mathcal{H}_{12} = {}_3\mathcal{H}_{12} = 0.$$

At η^*,

These three constraints define an $(n-3)$-dimensional submanifold in η. If $n = 3$, then the degeneracy defines an isolated point in η.

For a system with time-reversal symmetry, the Hamiltonian $\mathcal{H}$ is real and $\mathrm{Im}\mathcal{H}_{12} = 0$. Hence, the subspace of degenerate points defines an $(n-2)$-dimensional submanifold of η. This behavior was recognized by von Neumann and Wigner [189]. Note that if we introduce the three parameters

$$u = \frac{1}{2}\,(\mathcal{H}_{11} - \mathcal{H}_{22})\,, \quad v = \mathrm{Re}\mathcal{H}_{12}, \quad w = \mathrm{Im}\mathcal{H}_{12},$$

then the eigenenergies in the vicinity of the degeneracy take a double-cone profile, as shown in Figure 10.2, with its apex at the degeneracy point, namely

$$E = E^* \pm \sqrt{u^2 + v^2 + w^2}$$

The double cone is called a diabolo (after a spinning toy of the same shape). The apex of this cone is called a diabolical point. [3]

10.2.4 Berry's Quantized Flux and Topological Invariant

The flux of Berry's curvature through a surface $\mathbf{S}$ remains a bona fide physical quantity on closed surfaces, such as a sphere or a torus, in which case the closed contour C becomes the empty set. The remarkable feature in this case is that the flux is quantized. For pedagogical reasons, we will consider the simple case of a sphere in three dimensions, $\mathbf{S} \equiv \mathbb{S}^2$. For regular and divergence-free curvature on the closed surface $\mathbb{S}^2$,

$$\int_{\mathbb{S}^2} \mathcal{F}(\eta) \cdot d\mathbf{S}$$

represents the flux of $\mathcal{F}$ across $\mathbb{S}^2$. The flux quantization is then expressed as

$$\mathcal{C}_1 = \frac{1}{2\pi} \int_{\mathbb{S}^2} \mathcal{F}(\boldsymbol{\eta}) \cdot d\mathbf{S},$$

where $\mathcal{C}_1$ is an integer $\in \mathbb{Z}$, called the Chern number of the first class. To demonstrate that $\mathcal{C}_1 \in \mathbb{Z}$, we shall assume that $\mathcal{F}(\eta)$ is singular at $\eta = 0$, and that $\mathbb{S}^2$ is the spherical surface centered at the origin (see Figure 10.3).

We cut this surface at the equator, $\eta_z = 0$, and consider the flux across the two open surfaces

$$\int_{\mathbb{S}^2} \mathcal{F}(\boldsymbol{\eta}) \cdot d\mathbf{S} = \int_{S_+} \mathcal{F}(\boldsymbol{\eta}) \cdot d\mathbf{S} + \int_{S_-} \mathcal{F}(\boldsymbol{\eta}) \cdot d\mathbf{S}$$

We notice that $C_+ = C_- = C$, but the surface normals $\hat{\mathbf{n}}$ have opposite orientations. From Stokes' theorem, we get

$$\int_{S_\pm} \mathcal{F}(\boldsymbol{\eta}) \cdot d\mathbf{S} = \pm \int_C \mathcal{A}_\pm(\boldsymbol{\eta}) \cdot d\eta$$

$$\int_{\mathbb{S}^2} \mathcal{F}(\boldsymbol{\eta}) \cdot d\mathbf{S} = \int_C \mathcal{A}_+(\eta) \cdot d\eta - \int_C \mathcal{A}_(\eta) \cdot d\eta$$

The upper and lower Berry connections $\mathcal{A}_\pm(\eta)$ may only differ by a gauge transformation. Since the right-hand side (rhs) of (10.26) is the difference of two Berry phases on the same path, it is necessarily an integer multiple of 2π.

The Chern number turns out to be a robust topological invariant, and is associated with observable phenomena, such as the integer quantum Hall effect. More recently, other topological invariants have emerged, such as the $\mathbb{Z}_2$, which classifies time-reversal symmetric insulators into disjoint trivial and topological types.

As we have outlined, the integrand $\mathcal{F}$ is the curl of the Berry connection $\mathcal{A}$, and, in general, $\mathcal{A}$ may not be a single-valued function globally on $\mathbb{S}^2$, but only on local patches, as will be described in example 1.

6.7.5 Extra Understanding of Geometrical Phases 2

10.3 Pedagogical Example 1: A Two-Level System

Pedagogically, studying this system accomplishes two goals. First, it is a simple model that demonstrates the basic concepts outlined earlier in this chapter, and reveals several important properties of the Berry phase. Second, it will emerge, in different physical guises, in the following chapters. The generic Hamiltonian of a two-level system takes the form

$$\mathcal{H} = -\mathbf{d}\cdot\boldsymbol{\sigma},$$

where σ represents the Pauli matrices and $\mathbf{d}\in\mathbb{R}^3$ vector space. [4] We parametrize $\mathbf{d}$ by its polar and azimuthal angles θ and φ as

$$\mathbf{d} = d\hat{\mathbf{n}}, \quad \hat{\mathbf{n}} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta).$$

The two eigenstates, with energies $\pm d$, are

$$|\psi_+(\mathbf{d})\rangle = \begin{pmatrix} \cos(\theta/2) \\ e^{i\varphi}\sin(\theta/2) \end{pmatrix} \quad |\psi_-(\mathbf{d})\rangle = \begin{pmatrix} -\sin(\theta/2) \\ e^{i\varphi}\cos(\theta/2) \end{pmatrix}.$$

We notice that the norm d does not affect the eigenvectors. Therefore, the parameter space is a two-sphere $\mathbb{S}^2$.

10.3.1 Patches and Transition Functions

We now choose two different gauges to write the ground state $|\psi_-(\mathbf{d})\rangle$:

$$\left|\psi_-^U\right\rangle = \begin{pmatrix} -\sin(\theta/2) \\ e^{i\varphi}\cos(\theta/2) \end{pmatrix} \quad \text{or} \quad \left|\psi_-^L\right\rangle = \begin{pmatrix} -e^{-i\varphi}\sin(\theta/2) \\ \cos(\theta/2) \end{pmatrix}.$$

Both states $\left|\psi_-^U\right\rangle$ and $\left|\psi_-^L\right\rangle$ describe the ground state. However, $\left|\psi_-^U\right\rangle$ is ill defined (singular) at $\theta=\pi$ (it displays a vortex at the south-pole $\Rightarrow$ value of φ ill defined), while $\left|\psi_-^L\right\rangle$ is singular at the north-pole. Thus, we have to introduce two patches on the sphere, shown in Figure 10.4, to obtain a smooth parameterization of the instantaneous eigenstates. Other gauges yield the singularity at a different point on the sphere, but a singularity is unavoidable. It is impossible to find a gauge that yields a smooth, nonsingular connection over the whole closed surface. Such singularity, often called obstruction, can be moved but not removed..[5] However, we can glue these two patches together via a gluing phase

$$\left|\psi_-^U\right\rangle = e^{it(\varphi)}\left|\psi_-^L\right\rangle \quad t(\varphi)=\varphi$$

along the equator.

10.3.2 Berry Connection, Curvature, and Phase

We now calculate the Berry connection and curvature for ψ_-^U and ψ_-^L

$$\nabla\left|\psi_-^U\right\rangle = -\frac{1}{d}\begin{pmatrix} \frac{1}{2}\cos\frac{\theta}{2} \\ \frac{1}{2}e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}\hat{\vartheta} + \frac{1}{d\sin\theta}\begin{pmatrix} 0 \\ ie^{i\phi}\cos\frac{\theta}{2} \end{pmatrix}\hat{\boldsymbol{\varphi}}$$

Hence

$$\begin{aligned}\left\langle\psi_-^U|\nabla\psi_-^U\right\rangle &= \frac{1}{2d}\left[\sin\frac{\theta}{2}\cos\frac{\theta}{2}\hat{\boldsymbol{\theta}} - \sin\frac{\theta}{2}\cos\frac{\theta}{2}\hat{\boldsymbol{\theta}} + 2i\frac{\cos^2(\theta/2)}{\sin\theta}\hat{\varphi}\right] \\ &= i\frac{2\cos^2(\theta/2)}{d\sin\theta}\hat{\varphi} = i\frac{1}{d}\cot\frac{\theta}{2}\hat{\varphi}\end{aligned}$$

and

$$\nabla \times \left\langle \psi_-^U | \nabla \psi_-^U \right\rangle = \frac{1}{d \sin\theta} \frac{\partial}{\partial \theta} \left[\sin\theta \frac{i \cos^2(\theta/2)}{d \sin\theta} \right] \hat{\mathbf{n}} = -i \frac{1}{2d^2} \hat{\mathbf{n}}.$$

We obtain

$$\mathcal{A} = \frac{1}{d} \hat{\varphi} \times \begin{cases} \cot(\vartheta/2) & \left| \psi_-^U \right\rangle \quad \text{singular at } \theta = 0, \\ \tan(\theta/2) & \left| \psi_-^L \right\rangle \quad \text{singular at } \theta = \pi, \end{cases}$$

$$\mathcal{F} = \frac{1}{2d^2} \hat{\mathbf{n}}.$$

The curvature is gauge invariant, while the connection is gauge dependent. The curvature for the upper state $|\psi_+(\mathbf{d})\rangle$ is $\mathcal{F} = -\frac{1}{2d^2}\hat{\mathbf{n}}$. Thus, parallel transport of the eigenstates $|\psi_-(\mathbf{d})\rangle$ and $|\psi_+(\mathbf{d})\rangle$ over the same loop in parameter space rotates them in opposite directions (Berry phases have opposite signs). They exhibit a twist akin to the Möbius strip.

One- and Two-Form Approach

Alternatively, we can use the one-form expression for the connection and

$$\begin{aligned} \mathcal{A} &= i \langle \psi | d\psi \rangle \\ &= i \langle \psi | \partial_\theta \psi \rangle \, d\theta + i \langle \psi | \partial_\varphi \psi \rangle \, d\varphi \\ \frac{\partial \psi_-}{\partial \theta} &= - \begin{bmatrix} (\cos\theta)/2 \\ e^{i\varphi}(\sin\theta)/2 \end{bmatrix}, \quad \frac{\partial \psi_-}{\partial \varphi} = \begin{bmatrix} 0 \\ ie^{i\varphi}(\cos\theta)/2 \end{bmatrix} \\ \frac{\partial \psi_+}{\partial \theta} &= \begin{bmatrix} -(\sin\theta)/2 \\ e^{i\varphi}(\cos\theta)/2 \end{bmatrix}, \quad \frac{\partial \psi_+}{\partial \varphi} = \begin{bmatrix} 0 \\ ie^{i\varphi}(\sin\theta)/2 \end{bmatrix} \end{aligned}$$

to obtain

$$\begin{aligned} \mathcal{A}_+ &= \langle \psi_+ | d\psi_+ \rangle = -\frac{1}{2}(1 - \cos\theta) d\varphi \\ \mathcal{A}_- &= \langle \psi_- | d\psi_- \rangle = -\frac{1}{2}(1 + \cos\theta) d\varphi \end{aligned}$$

The corresponding Berry curvature is

$$\begin{aligned} \mathscr{F}_{\theta\varphi} &= (\partial_\theta \mathcal{A}_\varphi - \partial_\varphi \mathcal{A}_\theta) \, d\theta \wedge d\varphi \\ \mathcal{F}^+_{\theta\varphi} &= -\frac{1}{2} \sin\theta d\theta \wedge d\varphi \\ \mathcal{F}^-_{\theta\varphi} &= \frac{1}{2} \sin\theta d\theta \wedge d\varphi \\ \mathcal{F}^+_{\theta\varphi} + \mathcal{F}^-_{\theta\varphi} &= 0 \end{aligned}$$

and the Chern numbers are

$$\mathcal{C}_\pm = \mp \frac{1}{2\pi} \int_{S^2} d\theta \sin\theta d\phi \frac{1}{2} = \mp 1.$$

In the integration of the Berry curvature over the parameters (θ, φ), we did not include an additional $\sin\theta$ factor that is required for a sphere. This is because we were not integrating over the surface of a sphere, but over a parameter domain shown in the figure. Here, the parameter space has the topology of a sphere $\mathbb{S}^2$, but not its metric. However, we should also note that

$$\mathcal{F}^\pm_{\theta\varphi} = \mp \frac{1}{2} \sin\theta d\theta \wedge d\varphi = \mp \frac{1}{2d^2} (dd\theta)(d \sin\theta d\varphi) \hat{\mathbf{d}}.$$

10.3.3 The Monopole: Degeneracy, Singularity, and Obstruction

If we write the curvature as $\mathcal{F} = \frac{g}{2d^2}\hat{\mathbf{n}}$, we find that it has the form of a magnetic monopole field of strength g at the origin, namely,

$$\frac{1}{2\pi}\int_{\mathbb{S}^2} \mathcal{F}\cdot d\mathbf{S} = g.$$

The corresponding Berry potential $\mathcal{A}$ also shows monopole behavior at $\mathbf{d} \equiv \mathbf{B} = 0$. As expected, the vanishing of the Hamiltonian at $d = 0$ ushers a doubly degenerate state - a singularity (see Figure 10.5).

We note that integrating over the solid angle $\Delta\Omega$ subtended by $\Delta\mathbf{S}$ yields a Berry phase $\gamma = g\Delta\mathbf{\Omega}/2$ proportional to half the subtended solid angle.

In fact, g cannot take arbitrary values: we calculate the Berry phase along a path C that does not contain the south pole

$$\gamma(C) = \oint_C \mathcal{A}\cdot d\ell = \int_{\Sigma(C)} \mathcal{F}\cdot d\mathbf{S} = \frac{g}{2}\Omega(\Sigma) \bmod 2\pi,$$

where $\Omega(\Sigma)$ is the solid angle subtended by the surface Σ that contains the north pole. If we now choose the surface $\tilde{\Sigma} = \mathbb{S}^2 - \Sigma$

$$\gamma(C) = -\int_{\tilde{\Sigma}(C)} \mathcal{F}\cdot d\mathbf{S} = -\frac{g}{2}(4\pi - \Omega(\Sigma)) \bmod 2\pi = \frac{g}{2}\Omega(\Sigma) \bmod 2\pi,$$

we find that $g \in \mathbb{Z}$. This integer measures the strength of the singularity (magnetic monopole), which resides in a site inaccessible to the quantum system. With this simple yet pedagogical procedure, we can ascertain that a nonvanishing Chern number $\mathcal{C}$ is intrinsically linked to the inability to choose a smooth gauge. In other words, only if we have to choose several patches that we glue together with a gauge transformation can $\mathcal{C}$ be nonzero.

10.4 Pedagogical Example 2: Molecular Aharonov-Bohm Effect

In this example, we consider the quantum motion of the combined electronic and ionic components of a molecule. Here, the slow motion of the ions presents an adiabatic time evolution of the electronic motion and allows the application of the Born-Oppenheimer approximation (BOA).

(???? this is a big chapter with many details, maybe I'll move it to cond matter later)

10.4.1 The Effective Ionic Hamiltonian

We start from the complete Hamiltonian $\mathcal{H}$ of an isolated $\mathcal{N}$-atom molecular system, and explicitly separate the ionic kinetic energy

$$\mathcal{H}(\mathbf{X},[\mathbf{x}]) = \frac{1}{2}\sum_{j=1}^{\mathcal{N}}\frac{\mathbf{P}_j^2}{2M_j} + \mathcal{H}_e(\mathbf{X},[\mathbf{x}]) + E_{\text{elastic}}(\mathbf{X})$$

where $[\mathbf{x}]$ denotes the electronic degrees of freedom, and $\mathbf{X} = [\mathbf{X}_1, ..., \mathbf{X}_j, ..., \mathbf{X}_{\mathcal{N}}]$ represents the ionic positions, with $\mathbf{X}_j$ the position vector of ion j.$\mathbf{P}_j = -i\hbar\nabla_{\mathbf{x}_j}$ is the canonical momentum conjugate to $\mathbf{X}_j$, and M_j the mass of ion j. Eelastic is the ionic elastic energy for the configuration $\mathbf{X}$.

We invoke the BOA by initially ignoring the ionic kinetic energy, and applying the adiabatic approximation, where the coupling between different electronic states can be neglected. Thus, the slowly varying $3\mathcal{N}$-dimensional ionic position vector $\mathbf{X}$ in $\mathcal{H}(\mathbf{X},[\mathbf{x}])$ is demoted to a classical parameter and identified with the slow parameter η. Moreover, we use the BOA ansatz and write the eigenfunctions of (10.28), $|\Psi(\mathbf{X},[\mathbf{x}])\rangle$, as the product $\langle[\mathbf{x}]|\xi(\mathbf{X})\rangle\chi(\mathbf{X})$, where ξ and χ denote the electronic and ionic wavefunction, respectively. We start with solving the electronic eigenvalue problem

$$\mathcal{H}_e(\mathbf{X},[\mathbf{x}])\,|\xi_n(\mathbf{X},[\mathbf{x}])\rangle = E_n(\mathbf{X})\,|\xi_n(\mathbf{X},[\mathbf{x}])\rangle$$

and determine the ground-state energy $E_0(\mathbf{X})$ and wavefunction $|\xi_0(\mathbf{X},[\mathbf{x}])\rangle$. Our goal is then to construct an effective Schrödinger equation for the ionic wavefunction $\chi(\mathbf{X})$ by integrating out the electronic degrees of freedom. We first consider the action of the canonical ionic momentum $\mathbf{P}$ on the product ansatz

$$\mathbf{P}|\xi(\mathbf{X},[\mathbf{x}])\rangle\chi(\mathbf{X}) = -i\hbar|\xi(\mathbf{X},[\mathbf{x}])\rangle\nabla_{\mathbf{X}}\chi(\mathbf{X}) - i\hbar\,|\nabla_{\mathbf{X}}\xi(\mathbf{X},[\mathbf{x}])\rangle\,\chi(\mathbf{X}).$$

We integrate over the electronic degrees of freedom by acting on both sides with $\langle\xi(\mathbf{X},[\mathbf{x}])|$. We obtain the effective ionic kinematic momentum Π acting on $\chi(\mathbf{X})$

$$\Pi\chi(\mathbf{X}) = [\mathbf{P} - i\hbar\,\langle\xi(\mathbf{X},[\mathbf{x}])|\nabla_{\mathbf{X}}\xi(\mathbf{X},[\mathbf{x}])\rangle\,\chi\chi(\mathbf{X}),$$

where Berry's connection is clearly recognizable. The electronic eigenvalue $E_0(\mathbf{X})$ of the ground state plays the role of a scalar potential for ionic motion. The effective Hamiltonian acting on $\chi(\mathbf{X})$ is given by

$$\mathcal{H}_{\text{eff}} = \frac{1}{2}\sum_j \frac{1}{M_j}\mathbf{\Pi}_j^2 + E_0(\mathbf{X}) + E_{\text{elastic}}\,(\mathbf{X}).$$

10.4.2 A Simple Example: The Trimer Molecule

The smallest molecular system that exhibits molecular Aharonov-Bohm effect is a trimer, with ionic coordinates $\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3)$. The simplest trimers, which we consider here, are of course the homonuclear ones, where symmetry plays a major role.

Structure of the Ground State

We focus on a trimer of monovalent atoms, such as H_3 or Na_3, where the occupied valence orbitals, $|A\rangle, |B\rangle$, and $|C\rangle$, are s-like.

We start with the molecule in the equilateral configuration of Figure 10.6, with $\mathcal{D}_{3\,\text{h}}$ symmetry. [7] Two of the valence electrons occupy a totally symmetric orbital (A_{1g} symmetry)

$$\left|\phi_{\text{A}_1\ \text{g}}\right\rangle = \frac{1}{\sqrt{3}}[|A\rangle + |B\rangle + |C\rangle].$$

The remaining unpaired electron occupies the next available orbital, which has E_{g} symmetry and is doubly degenerate. [8] In a simple tight-binding scheme, a possible basis is the two-dimensional manifold

$$\left|\phi^1_{\text{E}_\text{g}}\right\rangle = \frac{1}{\sqrt{2}}[|B\rangle - |C\rangle], \quad \left|\phi^2_{\text{E}_\text{g}}\right\rangle = \frac{1}{\sqrt{6}}[2|A\rangle - |B\rangle - |C\rangle].$$

These orbitals are shown in Figure 10.7. The fact that the Hamiltonian is time reversal invariant and the wavefunctions vanish at infinity guarantees that the orbitals may always be chosen as real.

When we distort the molecule from its equilateral configuration, the doublet is linearly split, and one of the two E_g components becomes energetically favored. The molecule is said

to undergo a Jahn-Teller distortion, where the electronic ground state in the BOA becomes nondegenerate.

The $E \otimes \varepsilon$ Jahn-Teller Problem

We shall start our study of this effect with describing the motion of the ions under $\mathcal{D}_{3\ \mathrm{h}}$ symmetry. We find three symmetry-adapted (normal) modes for small oscillations of the trimer molecule, shown in Figure 10.8:

(i) A breathing mode of A_{1g} symmetry. It is totally symmetric and cannot remove the electronic doublet degeneracy

(ii) An E_{g} doubly degenerate mode. It can lift the electronic degeneracy, and is compatible with coupling to the electronic doublet and engendering invariant terms in the Hamiltonian, linear in the symmetry-adapted displacements. The vibrational doublet, in fact, drives the dynamical Jahn-Teller effect [9].

The ionic motion lifts the electronic degeneracy. This fulfills the assertion of the Jahn-Teller theorem that in the presence of electronic degeneracy, there should be distorted ionic configurations of lower energy than the symmetric one.

Solving the One-Electron Problem

Within the Born-Oppenheimer procedure, we write

$$\Psi([\mathbf{x}], \mathbf{X}) = \chi(\mathbf{X})\xi([\mathbf{x}], \mathbf{X}))$$

and we initially neglect the ionic kinetic and elastic energies in $\mathcal{H}$. The remaining component is the electronic Hamiltonian having the form

$$\mathcal{H}_e(\mathbf{X}, \mathbf{x}) = T_e + V(\mathbf{X}, \mathbf{x})$$

for the one-electron case. T_ε is the electronic kinetic energy. The electron-ion potential V is expressed in terms of the "parametric" ionic positions $\mathbf{X}$ and the one-electron degrees of freedom $\mathbf{x}$.

For infinitesimal vibrational displacements, $\mathbf{X} = \mathbf{X}_0 + \Delta\mathbf{X}$, where $\mathbf{X}_0$ represents the equilibrium configuration with $\mathcal{D}_{3\ \mathrm{h}}$ symmetry. We expand the potential V to linear terms in $\Delta\mathbf{X}$:

$$\mathcal{H}_e(\mathbf{X}, \mathbf{x}) \simeq T_e + V\left(\mathbf{X}_0, \mathbf{x}\right) + \nabla_{\mathbf{X}} V|_{\mathbf{X}=\mathbf{X}_0} \cdot \Delta\mathbf{X}$$

As we have shown in Chapter 6, we carry out a unitary transformation to normal (or symmetry-adapted) coordinates $\mathbf{X} \to \mathbf{Q}$, and obtain

$$\begin{aligned}\mathcal{H}_e(\mathbf{Q}, \mathbf{x}) &= T_e + V\left(\mathbf{X}_0, [\mathbf{x}]\right) + \sum_\alpha \nabla_{\mathbf{Q}_\alpha} V \cdot \mathbf{Q}_\alpha \\ &= T_e + V\left(\mathbf{X}_0, \mathbf{x}\right) + \sum_\alpha \sum_{\ell=1}^{d_\alpha} K_{\alpha\ell} Q_\alpha^\ell = \mathcal{H}_e^{(0)} + \mathcal{H}'\end{aligned}$$

where $\mathbf{Q}_\alpha$ is a normal mode coordinate belonging to the irreducible representation (irrep) α and d_α is the irrep dimension, or its degeneracy. In the trimer case, the relevant irrep is E_g with $d_{\mathrm{E}_8} = 2$, yielding

$$\begin{aligned}\mathcal{H}_e &= \frac{\mathbf{p}^2}{2m_e} + V\left(\mathbf{x}; \mathbf{X}_0\right) + \mathcal{V}_1(\mathbf{x})Q_1 + \mathcal{V}_2(\mathbf{x})Q_2 \\ &= \mathcal{H}_e^{(0)} + \mathcal{V}_1(\mathbf{x})Q_1 + \mathcal{V}_2(\mathbf{x})Q_2\end{aligned}$$

where we dropped the subscript E_g. Diagonalization of $\mathcal{H}_e^{(0)}$ yields the solutions $|\xi_j\left(\mathbf{X}_0, \mathbf{x}\right)\rangle$ of the adiabatic electronic problem for the equilateral ionic configuration. However, since $\mathcal{H}_e^{(0)}$ has

the $\mathcal{D}_{3\ \mathrm{h}}$ symmetry, the ground-state wavefunction is still expressed in terms of an $A_{1\ \mathrm{g}}$ singlet and an E_{g} doublet: $\left|\phi_{\mathrm{A}_{1\ \mathrm{g}}}\right\rangle, \left|\phi^1_{\mathrm{E}_g}\right\rangle, \left|\phi^2_{\mathrm{E}_g}\right\rangle$.

Treating the interaction as a degenerate perturbation problem, we evaluate the matrix elements as 10

$$\left\langle\phi^1|\mathcal{V}(\mathbf{x})|\phi^1\right\rangle = -K, \quad \left\langle\phi^2|\mathcal{V}(\mathbf{x})|\phi^2\right\rangle = K, \quad \left\langle\phi^1|\mathcal{V}(\mathbf{x})|\phi^2\right\rangle = \left\langle\phi^2|\mathcal{V}(\mathbf{x})|\phi^1\right\rangle = K,$$

where we again dropped the subscript E_g. Expressing the electron eigenket in the form

$$\xi'(\mathbf{x},\mathbf{Q}) = A_1(\mathbf{Q})\phi^1(\mathbf{x},\mathbf{Q}) + A_2(\mathbf{Q})\phi^2(\mathbf{x},\mathbf{Q})$$

we obtain

$$\begin{pmatrix} -KQ_1 & KQ_2 \\ KQ_2 & KQ_1 \end{pmatrix} \Rightarrow \mathcal{E}_\pm = \pm K\sqrt{Q_1^2+Q_2^2}$$

Next, we transform the coordinates in $Q_1 - Q_2$ parameter space to polar form (Q,φ):

$$Q_1 = Q\cos\varphi, \text{ and } Q_2 = Q\sin\varphi$$

as shown in Figure 10.9, and obtain

$$KQ\begin{pmatrix} -\cos\varphi & \sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} = KQ\left(\sin\varphi\sigma_x - \cos\varphi\sigma_z\right),$$

where σ_x and σ_z are the Pauli matrices. The eigenenergies become

$$\mathcal{E}_\pm = \pm KQ.$$

The rhs of (10.32) shows that the coupling to the vibronic modes in the electronic problem can be mapped onto a spin- 1/2 problem. We can then write the eigenkets as

$$\begin{cases} |\xi_-\rangle = \frac{1}{\sqrt{2}}\left[\cos(\varphi/2)\,|\phi^1\rangle - \sin(\varphi/2)\,|\phi^2\rangle\right] \\ |\xi_+\rangle = \frac{1}{\sqrt{2}}\left[\sin(\varphi/2)\,|\phi^1\rangle + \cos(\varphi/2)\,|\phi^2\rangle\right] \end{cases}$$

The eigenkets $|\xi_\pm\rangle$are real and double-valued in the angle φ. We find that although the Hamiltonian is periodic in φ, the electronic wavefunctions are antiperiodic:

$$|\xi_\pm(2\pi)\rangle = -\,|\xi_\pm(0)\rangle\,.$$

We can also view the sign change in the electronic eigenstates, as a result of varying the angle φ along a closed loop encircling the origin in the ionic configuration parameter space, shown in Figure 10.9, a possible holonomy. This behavior is demonstrated in Figure 10.10. As we will see, this is characteristic of a cyclic pseudorotation.

The sign change in the state of a two-level (fermionic) system under a 2π rotation, referred to as spinor behavior, [11] was known since the early days of quantum mechanics, but we shall show that Berry's formulation brings a new insight, namely, a special case of the geometric phase. However, to start with, the reality of the wavefunctions leads to the vanishing of Berry's geometric vector potential, $(\xi_\pm\,|\nabla_Q|\,\xi_\pm\rangle = 0$.

(??? there was a cool picture here with triangles....)

The double-valued eigenstates of (10.33) may appear disturbing and unphysical. However, this problem can be remedied in two ways. We can apply a gauge transformation that renders the wavefunctions complex, but single-valued. Or, we require that the ionic wavefunction be quantized using antiperiodic boundary conditions. Note that the eigenstate of the total molecular system, $\Psi(\mathbf{x},\mathbf{Q})$, must be single-valued, of which the electronic term is only one factor.

10.4.3 Molecular A haronov-Bohm effect (MABE)

Before describing the molecular Aharonov-Bohm effect, we will briefly describe the original Aharonov-Bohm effect (ABE) [6], for the sake of clarity and completeness. The Aharonov-Bohm Effect In the simplest description of the Aharonov-Bohm effect, an electron is placed outside a solenoid with infinite extension in the z-direction (see Figure 10.11). The region inside the solenoid is inaccessible to the electron. For simplicity, we consider the case where the electron is confined to a circular rail of radius a, in the $x-y$ plane, as shown in figure. If the magnetic flux through the solenoid is Φ, then the vector potential at the rail will be

$$A_\varphi = \frac{\Phi}{2\pi a}.$$

The corresponding Hamiltonian is

$$\mathcal{H} = \frac{\hbar^2}{2m_e}\left(\frac{i}{a}\frac{d}{d\varphi} + \frac{e}{\hbar c}A_\varphi\right)^2 = -\frac{\hbar^2}{2m_e}\left(\frac{d}{d\varphi} - i\frac{\Phi}{\Phi_0}\right)^2,$$

where $\Phi_0 = 2\pi\hbar c/e = hc/e$ is the flux quantum. The single-valued eigenfunctions satisfying periodic boundary conditions are $\psi(\varphi) \propto \exp[i\ell\varphi], \ell$ integer, with eigenenergies

$$E_\ell = \frac{h^2}{2m_e a^2}\left(\ell + \frac{\Phi}{\Phi_0}\right)^2$$

which clearly demonstrates that the energy quantization may have a noninteger quantum number whose value depends on the solenoid flux! Moreover, we note that for Φ not equal to integer multiples of Φ_0, energies for ℓ values that have the same magnitude but differ in sign are not degenerate. The canonical and kinematic angular momenta differ, so that clockwise and counterclockwise directions have different speeds for a given value of $|\ell|$. The reason is that the vector field $\mathbf{A}$ causes the phase of the electron wavefunction to change as the wave circulates on the ring. To satisfy the boundary condition, this phase change, in turn, results in higher or lower kinematic momentum.

The key to the Aharonov-Bohm effect is the vector potential $\mathbf{A}(\mathbf{x})$. Outside the solenoid $\mathbf{B} = \nabla \wedge \mathbf{A} = 0$, but $\mathbf{A} \neq 0$ because for any closed loop surrounding the solenoid we have a nonzero integral

$$\oint_C \mathbf{A} \cdot d\boldsymbol{\ell} = \int_{\substack{\text{including}\\ \text{solenoid}}} \mathbf{B} \cdot d\mathbf{s} = \Phi$$

Thus, locally, $\nabla \wedge \mathbf{A} = 0$ means that the vector potential is a gradient of some function, and we may gauge it away

$$\mathbf{A}(\mathbf{x}) \to \tilde{\mathbf{A}}(\mathbf{x}) = \mathbf{A}(\mathbf{x}) - \nabla\xi(\mathbf{x}) = 0$$

but, globally, no single-valued $\xi(\mathbf{x})$ can gauge away the vector potential. [12]

To bring out the physics behind the ABE, we consider an electron beam being split at $\mathbf{x}$, and the two components travel along paths 1 and 2, of equal lengths, as shown in Figure 10.12. When they recombine at $\mathbf{x}'$, they have acquired different phases. We have two separate and

different gauge transforms $-\xi_1(\mathbf{x})$ that gauges away $\mathbf{A}(\mathbf{x})$ along path 1, and $\xi_2(\mathbf{x})$ that gauges away $\mathbf{A}(\mathbf{x})$ along path 2:

$$\Delta\xi|_{\text{path1}} - \Delta\xi|_{\text{path2}} = \oint_{\text{cloosed}} \mathbf{A}\cdot d\boldsymbol{\ell} = \Phi.$$

Gauge Transformation of Electronic States For pedagogical reasons, we shall use a gauge transformation to remove the doublevaluedness, and we write

$$|\xi_{\pm}(\mathbf{Q},\mathbf{x})\rangle \to \exp(i\varphi/2)\,|\xi_{\pm}(\mathbf{Q},\mathbf{x})\rangle$$

Such a transformation requires the addition of a gauge potential to the Hamiltonian. As we will show, the present case requires the introduction of a vector potential

$$\nabla \to \nabla - i(\hat{\varphi}/2Q)$$

This vector potential gives rise to a fictitious magnetic field (a flux tube) confined to the origin. Consequently, the $E\otimes\varepsilon$ system may be regarded as an analog of the AharonovBohm effect. Indeed, Mead has dubbed this the molecular Aharonov-Bohm effect [128]. As in BOA, the eigenstates acquire a phase γ from the vector potential.

- Berry's connection and phase

We start with calculating Berry's connection for the single-valued $\xi(\mathbf{Q},\mathbf{x})$ of (10.34). With $\nabla_Q = \left(\frac{\partial}{\partial Q}, \frac{1}{Q}\frac{\partial}{\partial\varphi}\right)$, we find

$$\begin{aligned}\nabla_Q\,|\xi_-\rangle &= \frac{\hat{\varphi}}{Q}\frac{\partial}{\partial\varphi}\left[e^{i\varphi/2}\left(-\sin\frac{\varphi}{2}\,|\phi^1\rangle + \cos\frac{\varphi}{2}\,|\phi^2\rangle\right)\right]\\ &= \frac{\hat{\varphi}}{2Q}e^{i\varphi/2}\left[i\,|\xi_-\rangle - |\xi_+\rangle\right]\end{aligned}$$

which yields

$$\langle\xi_-|\nabla\xi_-\rangle = \left[0, \frac{i}{2Q}\right] \Rightarrow \mathcal{A}_Q = i\,\langle\xi_-|\nabla\xi_-\rangle = -\frac{1}{2Q}\hat{\varphi}$$

and Berry's phase $\gamma_A(C)$ is given by

$$\gamma_A(C) = \oint_C \mathcal{A}_Q\cdot d\mathbf{l}_Q = \int_0^{2\pi}\left(-\frac{1}{2Q}\right)Q d\varphi = -\pi.$$

Quantization of Ionic Motion: Pseudorotations

- Effective scalar potential

Having determined the electronic energy contribution to be $\mathcal{E}_{\pm} = \pm KQ$, we now turn to the vibrational (slow motion) problem. The elastic energy of the vibration modes Q_1 and Q_2 is

$$E_{\text{elastic}}\,(\mathbf{Q}) = \frac{\kappa}{2}\left(Q_1^2 + Q_2^2\right) = \frac{\kappa}{2}Q^2,$$

where the two modes have the same effective spring constant κ since they are degenerate. The potential energy experienced by the molecular ion system becomes

$$\frac{\kappa}{2}Q^2 - KQ,$$

with $Q \geq 0$ in polar coordinates. This is just the Born-Oppenheimer surface of the JahnTeller split doublet shown in Figure 10.13:

- It is a double-valued function.

- It has a degeneracy at $Q = 0$ (the point of zero distortion), together with a conical intersection.

- The double cone is just a diabolo, and the degeneracy point a diabolical.

- Near the origin, the adiabatic approximation breaks down, and the origin becomes a singularity of the Born-Oppenheimer procedure.

- The domain of Q is not simply connected, because of the singularity at the origin (an obstacle).

- The lowest sheet has a continuum of minima, a circular valley of radius $Q_0 = K/\kappa$, $E_- = -K^2/2K$, where a classical particle travels freely.

Nothing exotic happens if the ionic motion can be considered as classic; but when we quantize the ionic degrees of freedom, Berry's connection arising from the gauge transformation in the electronic wavefunction gives rise to half-order quantum numbers. The ionic system becomes fermionic!

- The eigenvalue problem

Substituting the total eigenket

$$|\Psi(\mathbf{r}, \mathbf{Q})\rangle = \chi(\mathbf{Q}) \, |\xi_-\rangle$$

in the eigenvalue equation and setting $\kappa = \mu\omega_Q^2$, where μ is the mode effective mass, we obtain

$$\left[\frac{\mathbf{P}^2}{2\mu} + \left(\frac{\mu\omega_Q^2}{2}Q^2 - KQ\right)\right] \times |\xi_-\rangle = E\chi \, |\xi_-\rangle$$

or $|\xi_-\rangle \, \frac{\mathbf{P}^2}{2\mu}\chi + i\hbar\nabla_Q \, |\xi_-\rangle \cdot \left(\frac{\mathbf{P}}{\mu}\chi\right) - \frac{\hbar^2}{2\mu}\chi\nabla_Q^2 \, |\xi_-\rangle + \left(\frac{\mu\omega_Q^2}{2}Q^2 - KQ\right)\chi \, |\xi_-\rangle = E_\chi \, |\xi_-\rangle$. Eliminating the electronic degrees of freedom, we get

$$\frac{\mathbf{P}^2}{2\mu}\chi + i\hbar \, \langle \xi_- \, |\nabla_Q| \, \xi_- \rangle \cdot \left(\frac{\mathbf{P}}{\mu}\chi\right) - \frac{\hbar^2}{2\mu} \, \langle \xi_- \, |\nabla_Q^2| \, \xi_- \rangle \, \chi + \left(\frac{\mu\omega_Q^2}{2}Q^2 - KQ\right)\chi = E\chi.$$

If we determine $\langle \xi_- \, |\nabla_Q^2| \, \xi_- \rangle$by operating on (10.35) with ∇_Q, we get

$$\langle \xi_- \, |\nabla_Q^2| \, \xi_- \rangle = \langle \xi_- \, |\nabla_Q \cdot \nabla_Q| \, \xi_- \rangle = \frac{1}{2Q^2}\frac{\partial}{\partial\varphi}e^{i\varphi/2} \left[i \, |\xi_-\rangle - |\xi_+\rangle\right] = -\frac{1}{2Q^2}.$$

Using the relations

$$\mathcal{A}_Q = i \, \langle \xi_- | \nabla \xi_- \rangle = -\frac{1}{2Q}\hat{\varphi}, \quad \nabla_Q = \left(\frac{\partial}{\partial Q}, \frac{1}{Q}\frac{\partial}{\partial\varphi}\right), \quad \nabla_Q^2 = \nabla_Q^2 + \frac{1}{Q^2}\frac{\partial^2}{\partial\varphi^2}$$

in (10.36), we obtain

$$\left[-\frac{\hbar^2}{2\mu}\nabla_{\mathbf{Q}}^2 + \frac{\hbar^2}{2\mu}\frac{1}{Q^2}\left(i\frac{\partial}{\partial\varphi}\right) + \frac{\hbar^2}{4\mu Q^2} + \left(\frac{\mu\omega_Q^2}{2}Q^2 - KQ\right)\right]\chi(\mathbf{Q}) =$$

$$\left[-\frac{\hbar^2}{2\mu}\nabla_Q^2 + \frac{\hbar^2}{2\mu Q^2}\left(-\frac{\partial^2}{\partial\varphi^2} + i\frac{\partial}{\partial\varphi}\right) + \frac{\hbar^2}{4\mu Q^2} + \left(\frac{\mu\omega_Q^2}{2}Q^2 - KQ\right)\right]\chi(\mathbf{Q}) =$$

$$\left[-\frac{\hbar^2}{2\mu}\nabla_Q^2 + \frac{\hbar^2}{2\mu Q^2}\left(i\frac{\partial}{\partial\varphi} + \frac{1}{2}\right)^2 + \frac{\hbar^2}{8\mu Q^2} + \left(\frac{\mu\omega_Q^2}{2}Q^2 - KQ\right)\right]\chi(\mathbf{Q}) = E\chi(\mathbf{Q})$$

- Quantized angular motion in Q-space: pseudorotations

Since χ has to be single-valued and periodic in φ, we set

$$\chi(\mathbf{Q}) = \eta(Q)e^{im\varphi}$$

so that the second term in (10.37) becomes

$$\frac{\hbar^2}{2\mu Q^2}\left(m-\frac{1}{2}\right)^2 = \frac{\ell^2\hbar^2}{2\mu Q^2}, \quad |\ell| = 1/2, 3/2, 5/2, ...$$

The pseudorotation term is obviously an ionic rotor in Q-space. But the angular energy is characterized by a half-integer quantum number ℓ, instead of the integer quantum number m. The lowest state with $\ell = \pm 1/2$ is an orbital doublet. This feature can be considered a manifestation of Berry's phase, which arises because we insisted that the electronic wavefunction be single-valued in Q-space!

The spectrum of (10.38) has the same structure as in ABE, if we identify the inaccessible flux Φ with half a flux quantum Φ_0, sometimes referred to as a π flux. There is no magnetic field in this problem; the flux is purely topological and can be regarded as an obstruction, since the ionic path cannot be contracted without crossing a degeneracy point. [13]

- Radial motion in Q-space

To complete the analysis of the molecular Aharonov-Bohm phenomenon, we consider here the radial motion. With

$$\nabla_Q^2 = \frac{1}{Q}\frac{\partial}{\partial Q}\left(Q\frac{\partial}{\partial Q}\right)$$

we write (10.37) in the form

$$\left[\frac{1}{Q}\frac{\partial}{\partial Q}\left(Q\frac{\partial}{\partial Q}\right) - \frac{A}{Q^2} - \left(\frac{\mu\omega_Q}{\hbar}\right)^2\left(Q-\frac{K}{\mu\omega_Q^2}\right)^2 + \frac{K^2}{\hbar^2\omega_Q^2} + \frac{2\mu E}{\hbar^2}\right]\eta(Q) = 0$$

where $A = \frac{\hbar^2}{2\mu Q^2}\left[\left(m-\frac{1}{2}\right)^2 + \frac{1}{4}\right]$ If we replace $\left(Q-\frac{K}{\mu\omega^2}\right)^2$ by Q^2, we have the radial equation of the isotropic twodimensional harmonic oscillator! Hence, (10.39) is the radial equation of a displaced isotropic oscillator, where the low-lying wavefunctions are centered on the potential minimum $Q_0 = \frac{K}{\mu\omega_Q^2}$, and concentrated in its trough. For these low-lying states, we can write

$$Q - \frac{K}{\mu\omega^2} = \Delta Q \Rightarrow \frac{\partial}{\partial \Delta Q} = \frac{\partial}{\partial Q}$$

with $\Delta Q \ll Q_0$. This allows us to set $Q \simeq Q_0$ in the first two terms of (10.39), so that (10.39) reduces to

$$\left[\frac{\partial^2}{\partial \Delta Q^2} - \left(\frac{\mu\omega_Q}{\hbar}\right)^2\Delta Q^2 + \frac{2\mu E'}{\hbar^2}\right]\eta(\Delta Q) = 0$$

which is just the equation of the one-dimensional harmonic oscillator. To visualize the behavior of this system, we first establish the analogy between the isotropic oscillator and circularly polarized light: in the latter, we have two oscillating linear electric fields that are spatially orthogonal; in the former, we have x and y oscillators. In the present system, we have two normal modes Q^1 and Q^2 that perform circular motion in $Q^1 - Q^2$ space. In real space, we have instantaneous linear superpositions of the two modes according to $Q^1 = Q\cos\varphi(t)$ and $Q^2 = Q\sin\varphi(t)$.

The vibrorotations, or pseudorotations, are depicted in Figure 10.14, with the degeneracy point represented by the equilateral triangle, and its morphing into pseudorotational distortions appears around the closed circular path.

О связи фазы Берри с дифференциальной геометрией

(тоже пропишу потом, иногда такой возникает вопрос)

Aharonov-Anandan Phase

Y. Aharonov and J. Anandan, "Phase change during a cyclic quantum evolution", Phys. Rev. Lett. 58 (1987) 1593-1596.

In 1987, Aharonov and Anandan [3] considered cyclic evolutions that are not restricted by an adiabatic condition and purposed an generalization of Berry's phase. This generalization is very important, because the adiabatic condition is never exactly fulfilled for real evolutions.

(??? If I need, I'll study it.)

6.7.6 Stationary Adiabatics

Метод Борна-Оппенгеймера

Постановка задачи для молекулы

Пусть гамильтониан квантовомеханической системы зависит от параметров, которые сами представляют собой квантомеханические степени свободы, которые тоже необходимо рассматривать с точки зрения стационарного уравнения Шрёдингера. Предположим, что в системе имеются «быстрые» степени свободы x_f и медленные» степени свободы x_s, то есть

$$\hat{H} = \hat{H}_s\left(\boldsymbol{x}_s\right) + \hat{H}_f\left(\boldsymbol{x}_f, \boldsymbol{x}_s\right)$$

то есть представляет собой сумму гамильтониана быстрой подсистемы $\hat{H}_f\left(x_f, x\right)$ (куда включено в том числе и её взаимодействие с медленной), который зависит от конкретного положения медленной как от параметров, и гамильтониана медленной подсистемы.

Каноническим примером, для которого впервые был развит адиабатический метод, является задача о квантовомеханическом описании молекулы. Молекула состоит из атомарных $x_s = \{R_i\}_{i=1}^{N_n}$ и электронных $x_f = \{r_i\}_{i=1}^{N_s}$ степеней свободы. Поскольку атомы в тысячи раз тяжелее электронов, то их квантомеханическое движение медленное, а движение электронов - быстрое.

Для молекулы гамильтониан нредставляет собой сумму кинетических энергий всех атомов и электронов, а также попарных Кулоновских энергий взаимодействия.

Разбиение гамильтониана в таком случае естественно следующее:

$$\hat{H}_s\left(\{\boldsymbol{R}_i\}\right) = \sum_{i=1}^{N_n} \frac{-\nabla^2_{\boldsymbol{R}_i}}{2M_i} + \sum_{i<j} \frac{Z_i Z_j e^2}{|\boldsymbol{R}_i - \boldsymbol{R}_j|}$$

$$\hat{H}_f\left(\{r_i\}, \{\boldsymbol{R}_j\}\right) = \sum_{i=1}^{N_e} \frac{-\nabla^2_{r_i}}{2m} + \sum_{i<j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} - \sum_{i=1}^{N_n}\sum_{j=1}^{N_e} \frac{Z_i e^2}{|\boldsymbol{R}_i - \boldsymbol{r}_j|}$$

О случаях, когда нужно учитывать квантовополевые эффекты атомов (?!?!?)

(то есть когда такая задача не работает?)

О случаях, когда нужно расчитать характеристики для конечной температуры (?!?!?)

(решаем при нулевой, дальше добавляем её как-то? методом Монте Карло что ли, отдав прогеру?)

адиабатическое разделение переменных

Логика метода очень сильно перекликается с нестационарной адиабатикой, разобранной ранее.

Если имеется сильное разделение временных масштабов, на которых «живут» различные подсистемы, то можно считать, что для «быстрой» подсистемы, «медленная» практически покоится.

Поэтому разумно решать для неё стационарное уравнение Шрёдингера, считая положение быстрой системы просто как параметр:

$$\hat{H}_f(x_f, x_s)\left|\psi_n^{(f)}(x_s)\right\rangle = \varepsilon_n^{(f)}(x_s)\left|\psi_n^{(f)}(x_s)\right\rangle$$

Таким образом мы находим полный набор состояний «быстрой» подсистемы $\psi_n^{(f)}(x_f, \{x_s\})$ и набор уровней энергии $\varepsilon_n^{(f)}(\boldsymbol{x}_s)$. Теперь, следуя логике нестационарной адиабатики, если «медленная» подсистема будет испытывать движение, то «быстрая» будет следовать мгновенным уровням энергии.

Таким образом, энергия $\varepsilon_n^{(f)}(\boldsymbol{x}_s)$ выступит в роли эффективной потенциальной энергии для движения медленной подсистемы.

Таким образом, после этого мы можем решить уравнение Шрёдингера для быстрой подсистемы, и тем самым завершая решение задачи.

Теперь схему конкретней.

Мы будем искать полное решение задачи в виде разложения по «мгновенным» собственным состояниям «быстрого» гамильтониана:

$$\Psi(x_f, x_s) = \sum u_n(x_s)\,\psi_n^{(f)}(x_f, \{x_s\})$$

Если мы сделаем такую подстановку в полное уравнение Шрёдингера, и спроецируем его на бра-вектор $\left\langle\psi_n^{(f)}\right|$, то мы получим следующее уравнение:

$$\sum_m \hat{H}_{nm}(x_s)\,u_m(x_s) + \varepsilon_n^{(f)}(x_s)\,u_n(x_s) = Eu_n(x_s), \quad \hat{H}_{nm}(x_s) = \left\langle\psi_n^{(f)}(x_s)\left|\hat{H}_s(x_s)\right|\psi_m^{(f)}(x_s)\right\rangle$$

Несмотря на внешнюю схожесть, $\hat{H}_{nm}(x_s)$ не является матричным элементом какого-то оператора, ведь функции $|\psi_n^{(f)}\rangle$ относятся к гильбертовому пространству быстрой подсистемы, а $\hat{H}_s$ -оператор, действующий на медленные степени свободы; поэтому $\hat{H}_{nm}(\boldsymbol{x}_s)$ остаётся оператором, действующим на медленные степени свободы.

С другой стороны, $\hat{H}_s(x_s)$ может содержать операторы типа градиентов по x_s и в этом смысле будет действовать на волновые функции $\left|\psi_m^{(f)}(\boldsymbol{x}_s)\right\rangle$ просто как дифференцирование по соответствующему параметру - именно поэтому $\hat{H}_{nm}(\boldsymbol{x}_s)$, вообще говоря, отлично от $\hat{H}_s(x_s)\,\delta_{nm}$. Однако в первом приближении его можно таковым считать, поскольку дифференцирование «быстрой» волновой функции по параметрам медленной системы, вообще говоря, содержит малость по параметру $\omega_{nm}^{(f)} \gg \omega_{nm}^{(s)}$(как будет показано нижу) -поэтому в ведущем приближении:

$$\left[\hat{H}_s(x_s) + \varepsilon_n^{(f)}(x_s)\right]u_n(x_s) = Eu_n(x_s)$$

Это и есть основное уравнение в адиабатическом приближении, и именно оно было озвучено ранее.

Разберём теперь поподробнее, на чём основываются сделанные приближения.

Переходы на другие состояния

До сих пор всё было точно, и полученное уравнение полностью эквивалентно исходному уравнению Шрёдингера.

Однако теперь, следуя логике из разобранной ранее нестационарной адиабатики, мы можем начать делать приближения.

Первое приближение заключается в том, что, как и ранее, если расстояние между соседними уровнями быстрой системы большое, то возбуждаться эти уровни не будут- что соответствует малости $\hat{H}_{n\neq m}$. Поступим в полной аналогии с нестационарной адиабатикой, когда мы оценивали выражение $\langle\psi_n|\partial_t\psi_m\rangle$:

$$\left\langle \psi_n^{(f)} \left| \left[\hat{H}_f\left(\boldsymbol{x}_f, \boldsymbol{x}_s\right), \hat{H}_s\left(\boldsymbol{x}_s\right) \right] \right| \psi_m^{(f)} \right\rangle \equiv \varepsilon_n^{(f)}\left(\boldsymbol{x}_s\right) \hat{H}_{nm}\left(\boldsymbol{x}_s\right) - \hat{H}_{nm}\left(\boldsymbol{x}_s\right) \varepsilon_m^{(f)}\left(\boldsymbol{x}_s\right)$$

Опять подчеркнём, что $\hat{H}_s\left(x_s\right)$ может содержать градиенты, действующие на x_s, и в этом смысле не коммутирует с $\varepsilon_n^{(f)}\left(\{x_s\}\right)$. Однако, если расстояние между уровнями достаточно большое $\omega_{nm}^{(f)} \gg \omega_{nm}^{(s)}$, то членом с коммутатором можно пренебречь и написать следующую оценку:

$$\hat{H}_{nm}\left(\boldsymbol{x}_s\right) \simeq \frac{\left\langle \psi_n^{(f)} \left| \left[\hat{H}_f\left(\boldsymbol{x}_f, \boldsymbol{x}_s\right), \hat{H}_s\left(\boldsymbol{x}_s\right) \right] \right| \psi_m^{(f)} \right\rangle}{\omega_{nm}^{(f)}\left(\boldsymbol{x}_s\right)}, \quad n \neq m$$

(сравните с формулой (5) предыдущего семинара.

Она была точной, в то время как тут мы пренебрегли коммутатором $\left[\hat{H}_{nm}\left(\boldsymbol{x}_s\right), \varepsilon_m^{(f)}\left(\boldsymbol{x}_s\right)\right]\Big)$. Опять-таки, покуда в системе нет вырождения или близких уровней, то оффдиагональными элементами $\hat{H}_{n\neq m}$ в ведущем порядке можно пренебречь.

Наконец, такая форма демонстрирует ещё один смысл адиабатического приближения.

Мы знаем, что если такой коммутатор равен нулю, то это означает, что в задаче разделяются переменные - достаточно независимо диагонализовать оба гамильтониана, и задача будет решена.

В этом смысле, стационарное адиабатическое приближение - это просто приближённое разделение переменных.

Диагональные элементы

Теперь разберёмся с диагональными элементами- на примере задачи Борна-Оппенгеймера, где интересующая нас часть гамильтониана, которая может действовать на параметр x_s, происходит просто из кинетической энергии $\hat{H}_s\left(\boldsymbol{x}_s\right) = \frac{\hat{p}_s^2}{2M}$. Тогда:

$$\left\langle \psi_n^{(f)} \left| \hat{p}_s^2 \right| \psi_n^{(f)} \right\rangle = \hat{p}_s^2 - 2 \cdot \boldsymbol{A}_n\left(\boldsymbol{x}_s\right) \hat{p}_s - \left\langle \psi_n^{(f)} | \nabla_s^2 \psi_n^{(f)} \right\rangle$$

где введена кривизна Берри (сравните с формулой (20) предыдущего семинара):

$$\boldsymbol{A}_n\left(\boldsymbol{x}_s\right) = i \left\langle \psi_n^{(f)}\left(\boldsymbol{x}_s\right) | \nabla_s \psi_n^{(f)}\left(\boldsymbol{x}_s\right) \right\rangle$$

Последнее слагаемое можно преобразовать:

$$\begin{aligned}\left\langle \psi_n^{(f)}|\nabla_s^2\psi_n^{(f)}\right\rangle &= -i\nabla_s A_n\left(x_s\right) - \left\langle \nabla_s\psi_n^{(f)}|\nabla_s\psi_n^{(f)}\right\rangle = \\ &= -i\nabla_s A_n\left(x_s\right) + \sum_k \left\langle \psi_n^{(f)}|\nabla_s\psi_k^{(f)}\right\rangle \left\langle \psi_k^{(f)}|\nabla_s\psi_n^{(f)}\right\rangle = \\ &= -i\nabla_s A_n\left(x_s\right) - A_n^2\left(x_s\right) + \sum_{k\neq n} \left\langle \psi_n^{(f)}|\nabla_s\psi_k^{(f)}\right\rangle \left\langle \psi_k^{(f)}|\nabla_s\psi_n^{(f)}\right\rangle\end{aligned}$$

Замечательно тут то, что первые два слагаемых, совместно с первыми двумя слагаемыми исходного выражения, собираются просто в комбинацию $\left(-i\nabla_s - A_n\left(x_s\right)\right)^2$. Последнее же слагаемое переписьвается как обычно через производные гамильтониана, и даст зависящую от координат добавку к эффективному гамильтониану медленной подсистемы.

Окончательно:

$$\left\langle \psi_n^{(f)}\left(\boldsymbol{x}_s\right)\left|\hat{\boldsymbol{p}}_s^2\right|\psi_n^{(f)}\left(\boldsymbol{x}_s\right)\right\rangle \equiv \left(\hat{\boldsymbol{p}}_s - \boldsymbol{A}_n\left(\boldsymbol{x}_s\right)\right)^2 + \sum_{k\neq n} \frac{\left|\left\langle \psi_n^{(f)}\left|\frac{\partial \hat{H}_f}{\partial \boldsymbol{x}_s}\right|\psi_k^{(f)}\right\rangle\right|^2}{\left(\omega_{nk}^{(f)}\left(\boldsymbol{x}_s\right)\right)^2}$$

Мь получили, что диагональный элемент $\hat{H}_{nn}\left(\boldsymbol{x}_s\right)$ в главном порядке действительно совпадает с просто $\hat{H}_s\left(x_s\right)$. Однако отличие заключается в дополнительном вкладе от фазы Берри, которая войдёт в эффективный гамильтониан медленных степеней свободы, и дополнительный вклад, являющийся просто добавкой к эффективной потенциальной энергии $\varepsilon_n^{(f)}\left(\boldsymbol{x}_s\right)$. Отметим, что его ещё можно переписать следующим образом:

$$\delta\varepsilon_n^{(f)}\left(\boldsymbol{x}_s\right) = \frac{1}{2M}\sum_{k\neq n} \boldsymbol{A}_{nk}\boldsymbol{A}_{kn}, \quad \boldsymbol{A}_{nk} = i\left\langle \psi_n^{(f)}\left(\boldsymbol{x}_s\right)|\nabla_s|\,\psi_k^{(f)}\left(\boldsymbol{x}_s\right)\right\rangle$$

Кривизна Берри входит в точности как обычный электромагнитный вектор-потенциал.

Любопытно, что он может модифицировать классические уравнения движения, добавив в них эффективное «магнитное поле», и вообще это некий нетривиальнь̆й топологический вклад в движение медленной подсистемы, который приходит от нетривиальной структуры «быстрых» волновых функций.

О случаях применения метода Борна-Опенгеймера (!??!)

О применениях в задачах про молекулы (!?!?!?)

(просто говорим, что переменные разделяются. серьезно, в этом и вся суть??? а иначе как бы было???)

Не может ли такое быть, что быстрая система влияет на медленную систему, как в маятнике Кпицы?

(вроде как мы фиксируем медленную систему и изучам быструю в ней, а может ли быть, что такой подход не работает, пусть и система явно делится на две такие части? Не знаю пока.)

6.7.7 Examples of Fast and Slow Subsystems by Migdal Krainov 1

Theory

Рассмотрим две подсистемы, одна из которых характеризуется большими, а другая - малыми частотами. Взаимодействие между подсистемами не предполагаетея малым.

Пусть ξ - совокупность координат медленной подсистемы. Гамильтониан всей системы имеет вид

$$H = H_1(x, \xi) + H_2(\xi),$$

где H_1 включает гамильтониан быстрой подсистемы и ее взаимодействие медленной подсистемой.

В предыдущем разделе мы считали, что движение медленной подсистемы классично: мы задавали траекторию $\xi = \xi(t)$ и вводили скорость ξ. Теперь это не будет предполагаться.

Введем систему собственных функций гамильтониана H_1:

$$H_1(x, \xi)\varphi_n(x, \xi) = \varepsilon_n(\xi)\varphi_n(x, \xi),$$

как это делалось и ранее. Решение всей задачи

$$H\Psi_\lambda = E_\lambda \Psi_\lambda$$

ищем в виде

$$\Psi_\lambda = \sum_{n'} u_{n'\lambda}(\xi)\varphi_{n'}(x, \xi).$$

Подставляя (2.40) в (2.39), имеем

$$(H_1 + H_2)\sum_n u_{n'\lambda}(\xi)\varphi_{n'}(x, \xi) = E_\lambda \sum_{n'} u_{n'\lambda}(\xi)\varphi_{n'}(x, \xi).$$

Умножим это равенство слева на $\varphi_n^*(x, \xi)$ и проинтегрируем по x, пользуясь ортогональностью функций $\varphi_n(x, \xi)$:

$$\int \varphi_n^*(x, \xi)\varphi_{n'}(x, \xi)dx = \delta_{nn'}$$

Получаем

$$(\varepsilon_n - E_\lambda)\, u_{n\lambda} + \int \varphi_n^* H_2 \sum_{n'} u_{n'\lambda}\varphi_{n'} dx = 0.$$

При этом для простоты предположено, что H_1 коммутирует с ξ. Далее, так как

$$H_2 u_{n'\lambda}\varphi_{n'} = \varphi_{n'} H_2 u_{n'\lambda} + [H_2, \varphi_{n'}]\, u_{n'\lambda},$$

то

$$(\varepsilon_n - E_\lambda)\, u_{n\lambda} + H_2 u_{n\lambda} = -\sum_{n'} \int \varphi_n'' \,[H_2, \varphi_{n'}]\, dx \cdot u_{n'\lambda}$$

Это соотношение аналогично соответствуюнему выражению в предыдущем разделе, только $i\xi^\circ \frac{\partial \varphi_n}{\partial \xi} = i\frac{d\varphi_n}{dt}$ заменяется коммутатором $[\mathrm{H}_2, \varphi_n]$.

В соотношении (2.41) можно перенести член с $n' = n$ налево:

$$\left\{ H_2 - \left(E_\lambda - \varepsilon_n - \int \varphi_n^* \,[H_2, \varphi_n]\, dx \right) \right\} u_{n\lambda} = -\sum_{n' \neq n} \int \varphi_n^* \,[H_2, \varphi_{n'}]\, dx \cdot u_{n'\lambda}$$

Это уравнение удобно для применения метода последовательных приближений. В нулевом приближении получаем уравнение

$$\left\{[H_2(\xi) - [E_\lambda - \varepsilon_n(\xi)]\right\} u^{(0)}_{n\lambda}(\xi) = 0.$$

Мы видим, что энергия быстрой подсистемы играет роль потенциальной энергии в эффективном гамильтониане меділенной подсистемы.

Колебательные уровни энергии молекулы

Оценим энергию колебаний молекулы. Для простоты мы напишем все выражения для иона молекулы водорода, хотя результаты без труда переносятся и на более сложные молекулы. Гамильтониан иона молекулы водорода имеет вид (в атомных единицах)

$$H = -\frac{1}{2}\Delta_r - \frac{1}{\left|r - \frac{1}{2}R\right|} - \frac{1}{\left|r + \frac{1}{2}R\right|} + \frac{1}{R} - \frac{1}{M}\Delta_R$$

Здесь M - масса протона, F-координата электрона, $\pm\frac{1}{2}R$ - координаты протонов (рис. 21). Ядра образуют медлениуг подсистему, а эпектрон - быструю. В обозначениях теории, развитой выше, примем за $H_1(x, \xi)$ гамильтониан

$$H_1(r, R) = -\frac{1}{2}\Delta_r - \frac{1}{\left|r - \frac{1}{2}R\right|} - \frac{1}{\left|r + \frac{1}{2}R\right|} + \frac{1}{R}$$

и за $H_2(\xi)$ гамильтониан

$$H_2(R) = -\frac{1}{M}\Delta_R$$

(конечно, 1/R можно было бы перенести в H_2). Введем

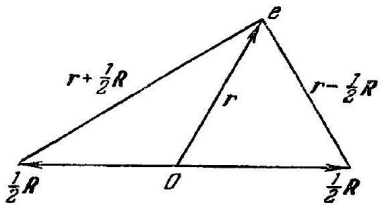


Рис. 21. Функцииг $\varphi_n(r, R)$, удовлетворяющие уравнению

$$H_1\varphi_n\{r, R) = \\ = \varepsilon_n(R)\varphi_n(r, R).$$

Они соответствуіот собственным функциям электрона при. фиксированном расстоянии между ядрами. Решение уравнения Шредингера с гамильтонианом Н имеет вид (см. стр. 94)

$$\Psi_\lambda = \sum_{n\nu} C^{n\nu}_\lambda \chi_{n\nu}(R)\varphi_n(r, R)$$

причем фупкиии $\chi_{n\nu}$ удовлетворнот уравнению

$$\left\{-\frac{1}{M}\Delta_R + \varepsilon_n(R)\right\}\chi_{n\nu}(R) = \omega_{n\nu}\chi_{n\nu}(R).$$

Ядра молекулы колеблются около некоторого среднего положения. Эти колебания имеют малую амплитуду. Поэтому для $\varepsilon_n(R)$ можно написать следующее приближенное выражение:

$$\varepsilon_n(R) \approx \varepsilon_n(R_0) + \frac{1}{2}\left(\frac{d^2\varepsilon_n}{dR^2}\right)_{R=R_0} \cdot (R-R_0)^2 .$$

Подставляя По $\varepsilon_n(R)$ в уравнение (2.44), получаем уравпоние Шредингера для трехмерного осциллятора. Следовательно, колсбателыные уровнц молекулы имеют вид

$$E_\lambda = \omega_{n\nu} = e_n(P_0) + \left(v + \frac{1}{2}\right)\omega_0,$$

гдє ω_0-частота классического осциллятора.

Найдем зависиность ω_0 от массы молекулы,

Из соотношения

$$\frac{1}{2}M\omega_0^2 (R-R_0)^2 = \frac{1}{2}\left(\frac{d^2\varepsilon_n}{dR^2}\right)_{R=R_0} \cdot (R-R_0)^2$$

вытекает, что

$$\omega_0 = \sqrt{\frac{1}{M}\left(\frac{d^2\varepsilon_n}{dR^2}\right)_{R=R_0}}.$$

Так как в атомных единицах электронные уровни $\varepsilon_n \sim 1$ и размеры молекулы $R_0 \sim 1$, то $\frac{d^2\varepsilon_n}{dR^2} \sim 1$ и, следовательно,

$$\omega_0 \sim \frac{1}{\sqrt{M}}.$$

Поскольку частоты электронных переходов $\omega_\pi \geqslant 1$, то мы Видим, ЧТО $\omega_0 \ll \omega_{9\pi}$.

Оценим амплитуду колебаний ядер. В основном состоянии осциллятора средние значения кинетической и потенциальной энергии совпадают: $\bar{T} = \bar{U} = E_0/2$ (E_0 - полная энергия), т. е.

$$\frac{1}{2}\left(\frac{d^2\varepsilon_n}{dR^2}\right)_{R=R_0} \cdot \overline{(R-R_0)^2} = \frac{1}{4}\omega_0.$$

Так как $\omega_0 \sim \sqrt{1/M}$, то величина среднего квадратичного отклонения ядра от положения равновесия имеет оценку

$$\sqrt{\overline{(R-R_0)^2}} \sim \frac{1}{\sqrt[4]{M}} \ll 1.$$

Покажем, что коэффициенты $C_\lambda^{n\nu}$ в выражении $\Psi_\lambda = \sum_{n\nu} C_\lambda^{n\nu}\chi_{n\nu}(R)\varphi_n(r,R)$, определяемые уравнением (2.42), можно вычислять методом последовательных приближений. Для этого оценим правую часть (2.42). Раскрывая коммутатор, получим члены следующего вида:

$$\left(\frac{1}{M}\chi_{n\nu}\varphi_n \Big| \frac{d\varphi_{n'}}{dR}\frac{d\chi_{n'}v'}{dR}\right), \quad \left(\frac{1}{M}\chi_{n\nu}\varphi_n \Big| \frac{d^2\varphi_{n'}}{dR^2}\chi_{n'v'}\right),$$

(члены вида $\left(\frac{1}{M}\chi_n, \varphi_n \Big| \varphi_{n'}\frac{d^2\chi_{n'v'}}{dR^2}\right)$ равны нулю). Оценим производные функции $\chi_{n\nu}$:

$$\frac{d\chi_{n_\nu}}{dR} \sim \frac{\gamma_{n_\nu}}{\sqrt{(R-R_0)^2}} \sim \sqrt[4]{(M}x_{n\nu}.$$

Поэтому из написанных двух типов членов самым большим будет первый: он порядка $1/\sqrt[4]{M^3}$. Итак, мы обосновали метод итераций в рассматриваемой задаче; каждая следующая итерация в $\sqrt[4]{M^3}$ раз меньше предыдущей.

кроме колебательных уровней, молекулы имеют также вращательные уровни. Частоты этих уровней обратно пропорциональны моменту инерции молекулы, т. е.

$$\omega_{\text{вран}} \sim 1/M.$$

Таким образом, электронные, колебательные и вращательные частоты находятся в следующем соотношении друг к другу:

$$\omega_{\text{вращ}} : \omega_{\text{кол}} : \omega_{\pi} = 1 : \sqrt{M} : M.$$

Возбуждение ядерных дипольных уровней быстрой частицей

Рассмотрим задачу о возбуждении атомного ядра при пролете мимо него быстрой заряженной частицы. В данном случае быстрая подсистема (налетающая частица) имеет сплошной спектр, а медленная (атомное ядро) - дискретный. Найдем решение, пользуясь адиабатической теорией возмущений. Для примснимости адиабатического приближения необходимо, чтобы время пролета частицы было мало гіо сравнению с существенными обратными частотами системы.

Сначала получим общне формулы для применения адиабатического приближения к задаче рассеяния. Введем собственные функции $\varphi_p(r, \xi_i)$ гамильтониана быстрой подсистемы $H_1 = T_r + V(r, \xi_i)$, где T_r - кинетическая энергия частицы, а $V(r, \xi_i)$ - ее взаимодействие с медленной подсистемой; ξ_i координаты медленной, r - быстрой подсистемы.

Таким образом, функции φp удовлетворяют уравнению

$$H_1 \varphi_p(r, \xi_i) = \varepsilon_p \varphi_p(r, \xi_i)$$

Энергия частицы $\varepsilon_p = p^2/2M$, т. е. не зависит от ξ_i, в отличне от случая дискретного спектра.

Ищем решение (2.45), имеющее асимптотический вид:

$$\varphi_{p\to\infty} \to e^{ipr} + \frac{f(\vartheta, \xi_i)}{r} e^{ipr}.$$

Поскольку ε_p не зависит от ξ_i, то уравнение для волновой функции медленной подсистемы (т. е. для ядра) будет таким же, как и без ε_p (только со сдвинутыми на ε_p собственными значениями):

$$H_2 \chi_n(\xi_i) = \omega_n \chi_n(\xi_i).$$

Ищем решение задачи в виде

$$\Psi_{pn} = \sum_n \int \frac{dp'}{(2\pi)^3} C_{pn}^{p'n'} \varphi_{p'} \chi_{n'}$$

причем коэффициенты $C_{pn}^{p'n'}$ подчиняются уравнению (см. (2.42))

$$(\omega_n - E_{p_0 n_0}) C_{p_n}^{p_0 n_0} = -\sum_{n'} \int \frac{dp'}{(2\pi)^3} (\varphi_p \chi_n [H_2, \varphi_{p'}] \chi_{n'}) C_{p_n}^{p'n'}.$$

Это уравиение можно решать последовательными приближениями. Пусть в начальный момент времени ($t = -\infty$) система находилась в состоянии ($\boldsymbol{p}_0, \boldsymbol{n}_0 \equiv 0$). Тогда в нулевом приближении

$$\Psi_{p_0 0}^{(0)} = C_0 \varphi_{p_0} x_0.$$

Точное решение должно иметь асимптотический вид:

$$\Psi \underset{r\to\infty}{\longrightarrow} e^{ip_0 r}\chi_0(\xi_i) + \frac{1}{r}\sum_n f_n(\vartheta) e^{ip_n r}\chi_n(\xi_i).$$

3 Зесь импульс p_n определяется законом сохранения энергии:

$$\varepsilon_{p_n} + \omega_n = \varepsilon_{p_0} + \omega_0.$$

Пренебрегая изменением энергии частицы, получим

$$\Psi \underset{r\to\infty}{\to} e^{ip_0 r}\chi_0(\xi_i) + \frac{e^{ip_0 r}}{r}\sum_n f_n(\vartheta)\chi_n(\xi_i).$$

Сравним с этим выражением асимптотический вид приближенного ренения $\Psi_{p_0\theta}^{(0)}$. Согласно (2.46) имеем

$$\Psi_{p_0 0}^{(0)} \underset{r\to\infty}{\longrightarrow} C_0\left(e^{ip_0 r}\chi_0(\xi_i) + \frac{e^{ip_0 r}}{r} f(\vartheta, \xi_i)\chi_0(\xi_i)\right) =$$
$$= C_0\left(e^{ip_0 r}\chi_0(\xi_i) + \frac{e^{ip_0 r}}{r}\sum_n (\chi_n f \chi_0)\chi_n\right).$$

Из сравнения (2.47) и (2.48) находим C_0 и амплитуды упругого и неупругого рассеяния:

$$C_0 = 1,$$
$$f_0(\vartheta) = (\chi_0(\xi_i)|f(\vartheta, \xi_i)|\chi_0(\xi_i))$$
$$f_n(\vartheta) = (\chi_n(\xi_i)|f(\vartheta, \xi_i)|\chi_0(\xi_i))$$

Используем полученные результаты для вычисления сечения возбуждения ядерных дигольных уровней быстрой заряженной частицей. Кулоновское взаимодействие пролетающей частицы с нуклонами ядра имеет вид (Z_1 - заряд частицы, Z_2 - заряд ядра):

$$V = Z_1\sum_i \frac{1}{|r - r_i|} = \frac{Z_1 Z_2}{r} + Z_1\frac{dr}{r^3} + ...$$

где d-динольный момент ядра. Этот потенциал можно представить в виде кулоновского, но со сдвинутым началом:

$$V \approx \frac{Z_1 Z_2}{\left|r - \frac{1}{Z_2}a\right|}$$

Для этого нужно, чтобы величина $a = d/Z_2$ была мала по сравнениио с существеными r, т. е. по сравнения с прицельным параметром $\rho : a \ll \rho$.

Следовательно, волновые функции φ_p будут кулоновскими волновыми функциями со сдвинутым аргументом:

$$\varphi_p(r, \xi_i) = \varphi_p^Q\left(r - \frac{1}{Z_2}d\right)\psi(\xi_i).$$

Выберем $\gamma(\xi_i)$ так, чтобы p имела асимптотический вид (2.46) :

$$\varphi_p(r,\xi_i) \underset{r\to\infty}{\to} \left\{\exp\left[ip\left(r-\frac{1}{Z_2}d\right)\right]+\frac{fQ(\vartheta)}{r}\exp\left[ip|r-\frac{1}{Z_2}d\right]\right\}\gamma(\xi_i),$$

где fQ - амплитуда кулоновского рассеяния. Для совпадения с (2.46) следует взять $\gamma(\xi_i) = e^{ipa}/Z_2$. Тогда

$$\varphi_p(r,\xi_i) \underset{r\to\infty}{\longrightarrow} e^{ipr}+\frac{e^{ipr}}{r}fQ(\vartheta)\exp\left[ip\left|r-\frac{1}{Z_2}d\right|+ipd\frac{1}{Z_2}-ipr\right]$$

Так как $\left|r-\frac{1}{Z_2}d\right| \approx r-\frac{1}{Z_2}\frac{dr}{r}$, то

$$\varphi_p(r,\xi_i) \underset{r\to\infty}{\longrightarrow} e^{ipr}+\frac{e^{ipr}}{r}fQ(\vartheta)\exp\left[iqd\frac{1}{Z_2}\right],$$

где $\boldsymbol{q} \equiv \boldsymbol{p}-\frac{\boldsymbol{p}}{r}r$ - векор, характеризубощий изменение импульса налетающей частицы цри столкновении. Поэтому согласно (2.49)

$$f_n(\vartheta) = f^Q(\vartheta)\left(x_n\left|\exp\left(iqd\frac{1}{Z_2}\right)\right|x_0\right).$$

Здесь f^Q - амплитуда кулоновского рассеяния.

Заметим, что сумма сечений для всех возбуждений равна

$$\sum_n |f_n(\vartheta)|^2 = \sum_n\left(x_0\left|\exp\left(-iqd\frac{1}{Z_2}\right)\right|\chi_n\right)\times\left(x_n\left|\exp\left(iqa\frac{1}{Z_2}\right)\right|x_0\right)\left|f^Q(\vartheta)\right|^2 = \left|f^Q(\vartheta)\right|^2,$$

т. е. равна сечению кулоновского рассеяния.

Если угол отклонения ϑ мал (малый переданный импульс), то из (2.50) получаем формулу теории возмущений:

$$f_n(\boldsymbol{\vartheta}) \approx f^Q(\boldsymbol{\vartheta})\left(\chi_n\left|\frac{i}{Z_2}qd\right|\chi_0\right),$$

амплитуда возбуждения пропорциональна дипольному матричному элементу.

Рассеяние протона на атоме водорода (перезарядка)

Рассмотрим рассеяние протона на атоме водорода, когда скорость протона много меньше скорости атомного электрона. В противоположность предыдущему случаю здесь дискретна быстрая подсистема, а у медленной подсистемы непрерывный спектр. Гамильтониан системы имеет вид

$$H = T_r-\frac{1}{\left|r-\frac{1}{2}R\right|}-\frac{1}{\left|r+\frac{1}{2}R\right|}+\frac{1}{R}-\frac{1}{M}\Delta_R.$$

В разделе 2.4 мы рассм атривали R как заданную функцию времени. Теперь мы рассматриваем налетающий протон и атом водорода как две взаимодействующие квантовомеханические системы.

Гамильтониан H симметричен к перестановке налетающей и покоящейся частиц ($\boldsymbol{r} \longrightarrow -\boldsymbol{r}$). Поэтому можно ввести симметричные и ағітисимметричные функции $\varphi_n^s(r,R)$ и $\varphi_n^a(r,R)$. Если нуклоны находятся далеко друг от друга, то электрон может находиться около одного либо около другого протона, и, следовательно,

$$\varphi_n^{s,a}(r,R) \underset{R\to\infty}{\longrightarrow} \frac{1}{\sqrt{2}}\left[\varphi_n^Q\left(r-\frac{1}{2}R\right)\pm\varphi_n^Q\left(r+\frac{1}{2}R\right)\right]$$

где в правой части стоят волновые функции атома водорода.

Предположим, что при сближении ядер не происходит пересечения термов. Тогда можно классифицировать их по тем состояниям, из которых они образовались.

Будем считать, что сначала электрон был около протона с координатой $R/2$, т. е. его волновая функция имеет вид

$$\varphi = \varphi^Q_{n_0}\left(r - \frac{1}{2}R\right).$$

Гамильтониан медленной подсистемы равен

$$H_2(R) = -\frac{1}{M}\Delta_R,$$

а его собственные функцни находятся из уравнения

$$\left[-\frac{1}{M}\Delta_R + \varepsilon^{s,a}_n(R)\right]\chi^{s,a}_{pn}(R) = E_p\chi^{s,a}_{pn}(R)$$

и имеют асимптотический вид

$$X^{s,a}_{pn}(R) \underset{R\to\infty}{\longrightarrow} e^{ipR} + \frac{f^{s,a}_n}{R}e^{ipR}.$$

В нулевом приближении решение задачи имеет вид (см. стр. 94)

$$\Psi_\lambda = C^{\lambda s}_{np}\varphi^s_n(r,R)\chi^s_{pn}(R) + C^{\lambda a}_{np}\varphi^a_n(r,R)\chi^a_{pn}(R)$$

Коэффициенты $C^{\lambda s}_{np}$ и $C^{\lambda a}_{np}$ определяются из асимптотического вида Ψ_λ :

$$\Psi_\lambda \underset{R\to\infty}{\to} \varphi^Q_{n_0}\left(r - \frac{1}{2}R\right)e^{ip_0R} + \left[f_1\varphi^Q_{n_0}\left(r - \frac{1}{2}R\right) + f_2\varphi^Q_{n_0}\left(r + \frac{1}{2}R\right)\right]\frac{e^{ip_0R}}{R},$$

где f_1 - амплитуда упругого рассеяния, а $f_2 \to$ амплитуда перезарядки.

Чтобы обеспечить асимптотический вид (2.53), нужно считать в (2.52)$p = p_0$ и $n = n_0$. Тогда волновая функцня (2.52) становится равной

$$\Psi_\lambda = C^s\varphi^s_{\pi_0}(r,R)\chi^s_{p_0n_0}(R) + C^a\varphi^a_{n_0}(r,R)\chi^a_{p_0n_0}(R)$$

и имеет асимптотический вид

$$\Psi_\lambda \underset{R\to\infty}{\longrightarrow} e^{ip_0R}\left(C^s\varphi^s_{n_0} + C^a\varphi^a_{n_0}\right) + \frac{1}{R}e^{ip_0R}\left(f^sC^s\varphi^s_{n_0} + f^aC^a\varphi^a_{n_0}\right)\cdot \quad (2.54)$$

Выражения (2.53) и (2.54) должны совпадать, т. е. нужно потребовать

$$C^s = C^a = \frac{1}{\sqrt{2}}.$$

Тогда из (2.54) находим

$$\begin{aligned}\frac{f^s\varphi^s_{n_0} + f^a\varphi^a_{n_0}}{\sqrt{2}} = \frac{1}{2}\Bigg\{f^s\left[\varphi^Q_{n_0}\left(r - \frac{1}{2}R\right) + \varphi^Q_{n_0}\left(r + \frac{1}{2}R\right)\right] + \\ + f^a\left[\varphi^Q_{n_0}\left(r - \frac{1}{2}R\right) - \varphi^Q_{n_0}\left(r + \frac{1}{2}R\right)\right]\Bigg\} = \\ = f_1\varphi^Q_{n_0}\left(r - \frac{1}{2}R\right) + f_2\varphi^Q_{n_0}\left(r + \frac{1}{2}R\right),\end{aligned}$$

Т. е.

$$f_1 = \frac{f_i^s + f^a\rfloor}{2}, \quad f_2 = \frac{f_1^s - f^a}{2}.$$

Таким образом, для нахождения амплитуды перезарядки f_2 и амплитуды упругого рассеяния f_1 необходимо вычислить амплитуды f^s и f^a. Чтобы найти их, нужно решить уравнение

$$\left[-\frac{1}{M}\Delta_R + \varepsilon_n^{s_n,a}(R)\right]\chi_{pn}^{s,a} = E_p\chi_{pn}^{s_s a}$$

с величинами $\boldsymbol{\varepsilon}_n^{s,a}(R)$, которые определяются из решения задачи об электроне в поле двух центров. В дальнейшем (стр. 151) мы найдем решение этой задачи в квазиклассическом приближении.

6.7.8 Examples of Fast and Slow Subsystems by Migdal Krainov 2

Рождение мягких квантов при рассеянии («инфракрасная катастрофа»)

Рассмотрим задачу о рождении мягких квантов при рассеянии частицы на ядре. Будем предполагать частицу нерелятивистской. Гамильтониан системы имеет вид

$$H = T + V - \frac{1}{c}pA + H_r.$$

Здесь T - кинетическая энергия частицы, V - рассеивающий потенциал, - $\frac{1}{c}pA$ - взаимодействие частицы с полем квантов, H_γ - гамильтониан поля квантов.

Предположим, что энергия квантов много меньше энергии частицы. Тогда движение частицы можно считать заданным и рассматривать только ту часть гамильтониана, которая содержит операторы, действующие на $\boldsymbol{\psi}$-функцию квантов. Гамильтониан γ-квантов за время столкновения, которое будем считать малым, меняется от величины $H_0 = H_\gamma - \frac{1}{c}p_0A$ до столкновения к величине $H_1 = H_\Upsilon - \frac{1}{c}p_1A$ после столкновения. Перейдем в систему координат, в которой частица до рассеяния покоилась. Тогда

$$H_0 = H_\gamma, \quad H_1 = H_\gamma - \frac{1}{c}qA,$$

где $q = p_1 - p_0$ - изменение импульса частицы в результате столкновения.

Возмущение $-\frac{1}{c}qA$ для малых частот становится большим, так как $A_{k\omega} \sim 1/\sqrt{\omega}$. Поэтому мы не будем пользоваться теорией возмущений, а используем только внезапность изменения гамильтониана γ-квантов.

Введем собственные фуикции χ_n гамильтониана H_0 и χ_n' гамильтоннана H_1. Предположим, что до столкновения система γ-квантов находилась в состоянии χ_0 Ввиду внезапности столкновения волновая функция системы χ_0 практически не изменяется. Следовательно, амплитуда перехода в состояние χ_n' равна $(\chi_n'|\chi_0)$ (см - стр. 75).

Представим гамильтониан электромагнитного поля $H_\gamma = \int\left(\frac{1}{8\pi c^2}\dot{A}^2 + \frac{1}{8\pi}(\mathrm{rot}\,A)^2\right)dr$ в виде суммы гамильтонианов отдельных осцилляторов поля. Для этого запишем векторный потенциал A в виде

$$A = \sum_{k\lambda}\sqrt{2\pi c^2}\eta_{k\lambda}\left(q_{k\lambda}\exp\left(ikr - i\omega_{k\lambda}t\right) + q_{k\lambda}^*\exp\left(-ikr + i\omega_{k\lambda}t\right)\right)$$

Здесь k - волновой вектор, λ - поляризация, $\omega_{k\lambda}$ - энергия квантов, $\eta_{k\lambda}$ - единичный вектор поляризации. Обозначая

$$q = Q + \frac{i}{\omega}P, q^* = Q - \frac{i}{\omega}P$$

и подставляя в H_γ, получим

$$H_r = \sum_{k\lambda} \frac{1}{2}\left(P^2 + \omega^2 Q^2\right)_{k\lambda}$$

В случае мягких квантов экспоненту e^{ikr} можно заменить единицей. Будем считать временны́е множители $\exp(\pm i\omega_{k\lambda}t)$ включенными в $q_{k\lambda}, q^*_{k\lambda}$. Опустим далее для простоты индексы $k\lambda$ при $q_{k\lambda}, q^*_{k\lambda}$. Тогда

$$A = \sum \sqrt{2\pi c^2}\eta \cdot 2Q.$$

(!?!??!!? подумаю еще про эту формулу???)

Гамильтониан квантов H_1 имеет вид

$$H_1 = \sum \left\{ \frac{1}{2}\left(P^2 + \omega^2 Q^2\right) - 2\sqrt{2\pi}(\eta g)Q \right\}.$$

Представим его в виде суммы осцилляторных гамильтонианов со смещенной координатой:

$$H_1 = \sum \left\{ \frac{1}{2}P^2 + \frac{1}{2}\omega^2(Q-\delta)^2 + \frac{1}{2}\omega^2\delta^2 \right\},$$

где $\delta = \frac{2\sqrt{2\pi}}{\omega^2}(\eta \boldsymbol{q})$.

Следовательно, волновые функции после столкновения $\chi'_n(Q)$ имеют вид осцилляторных функций, но со смещенной координатой:

$$\chi'_n(Q) = \chi_n(Q-\delta).$$

Таким образом, амплитуда перехода в состояние $x_n^{\dot{n}}$ имеет вид

$$C_n = \int \chi_n(Q-\delta)\chi_0(Q)dQ.$$

Предельные случаи

Рассмотрим сначала два предельных случая - малые и большие δ по сравнению с амплитудой нулевых колебанй. Если δ мало, то из $C_n = \int \chi_n(Q-\delta)\chi_0(Q)dQ$ /следует

$$C_n \approx -\delta \int \frac{\partial \chi_n}{\partial Q}\chi_0 dQ = i\delta(P)_{0n}$$

где P - оператор импульса. Он имеет отличные от нуля матричные элементы лишь для изменения числа квантов на единицу: $(P)_{01} = \frac{1}{2}\sqrt{\omega}$. Поэтому вероятность испускания одного кванта равна $w_1 = \frac{1}{4}\omega\delta^2 = \frac{2\pi}{\omega^3}(\eta q)^2\cdot$ Эта формула совпадает с результатом обычной теории возмущений.

Оценим матричный элемент $C_n = \int x_n(Q-\delta)\chi_0(Q)dQ$, когда смещение δ много больше амплитуды колебаний осциллятора. Для этого воспользуемся квазиклассическим выражением для функции x_n (см. 1.1 и 3.1) :

$$\chi_n(Q) = \frac{a_n}{\sqrt[4]{E_n - 1/2Q^2}} \cos\left(\int \sqrt{E_n - 1/2Q^2}dQ - \frac{\pi}{4}\right)$$

Для простоты здесь частота осциллятора ω взята равной единице. Результаты легко переносятся на случай $\omega \neq 1$. Нормировочный множитель a_n порядка единицы. Действительно,

$$1 = \int x_n^2 dQ \sim \frac{a_n^2}{\sqrt{E_n}} l_n \sim \frac{a_n^2}{\sqrt{E_n}}\frac{\sqrt{E_n}}{\omega}$$

Поэтому

$$C_n \sim \int \frac{\exp(-Q^2)}{\sqrt[4]{E_n - 1/2(Q-\delta)^2}} \cos\left(\int \sqrt{E_n - \frac{1}{2}(Q-\delta)^2} dQ - \frac{\pi}{4}\right) dQ$$

Так как величина δ, по предположению, много больше амплитуды нулевых колебаний, то можно под знаком корня в (2.65) пренебречь членом $Q^2/2$. Обозначим $E_n - \delta^2/2 \equiv \Delta E$ и заменим переменную интегрирования $Q : \Delta E/\delta + Q = x$. Тогда из (2.65) находим:

$$C_n \sim \int_0^\infty \frac{\cos\left(\delta^{1/2} x^{2/2}\right)}{\sqrt[4]{\delta x}} \exp\left(-x^2 + 2x\frac{\Delta E}{\delta}\right) dx \exp\left[-\left(\frac{\Delta E}{\delta}\right)^2\right]$$

Значения x, существенные в этом интеграле, соответствуют аргументу косинуса порядка единицы, т. е. имеют порядок величины $x \sim \delta\delta^{-1/2}$. Поэтому

$$C_n \sim \frac{1}{\sqrt[4]{\delta}} \frac{1}{\sqrt[12]{\delta}} \delta^{-1/3} \exp\left[-\left(\frac{\Delta E}{\delta}\right)^2\right] \sim \frac{1}{\sqrt{\delta}} \exp\left[-\left(\frac{\Delta E}{\delta}\right)^2\right],$$

$$|C_n|^2 \sim \frac{1}{\delta} \exp\left[-2\left(\frac{\Delta E}{\delta}\right)^2\right].$$

Таким образом, распределение вероятности испускания квантов имеет вид гауссовой кривой с максимумом $w_{\max} \sim 1/\delta$ и шириной $\Delta E \sim \delta$ около значения $E = \delta^2/2$. Это значение, как нетрудно видеть, совпадает с энергией классического осциллятора, начало координат которого внезапно сдвинуто на величину δ.

Случай произвольных δ

Теперь перейдем к вычислению C_n для произвольных δ. Вычислим сначала вероятность того, что не будет рождено ни одного кванта данного типа, т. е.

$$w_0 = \left|\int x_0(Q-\delta) x_0(Q) dQ\right|^2.$$

Так как волновая функция основного состояния осциллятора имеет вид

$$x_0(Q) = \sqrt[4]{\frac{\omega}{\pi}} \exp\left(-\frac{1}{2}\omega Q^2\right),$$

то

$$w_0 = \left|\sqrt{\frac{\omega}{\pi}} \int_{-\infty}^{\infty} \exp\left(-\omega Q^2 - \frac{1}{2}\omega\delta^2 + \omega Q\delta\right) dQ\right|^2 =$$

$$= \exp\left(-\frac{1}{4}\omega\delta^2\right) = \exp\left[-\frac{2\pi}{\omega^3}(q\eta)^2\right].$$

Восстановим теперь значки $\boldsymbol{k}, \lambda$. Тогда

$$\mathbf{0}_0^{k\lambda} = \exp\left[-\frac{2\pi}{\omega_{k\lambda}^3}\left(q\eta_{k\lambda}\right)^2\right]$$

- вероятность того, что не будет излучен ни один квант k, λ.

Вероятность того, что вообще не родится ни одного кванта ни в каком состоянии, равна

$$W_0 = \prod_{k\lambda} w_0^{k\lambda} = \exp\left[-\sum_{k\lambda} \frac{2\pi}{\omega_{k\lambda}^3} \left(q\eta_{k\lambda}\right)^2\right].$$

Для вычисления W_0 нужно найти сумму

$$\sum_{k\lambda} \frac{2\pi}{\omega_{k\lambda}^3} \left(q\eta_{k\lambda}\right)^2 = \sum_{\lambda} 2\pi \left(q\eta_{k\lambda}\right)^2 \int \frac{\omega^2 d\omega d\Omega}{(2\pi)^3 c^3 \omega^3}.$$

Мы видим, что при малых частотах это выражение логарифмически расходится. Следовательно, (???? как это следует?? разве не должна быть бесконечная вероятность????) $W_0 = 0$, т. е. любое торможение всегда будет сопровождаться излучением мягких квантов.

Вычислим матричный элемент $C_n = \int \chi_n(Q-\delta)\chi_0(Q)dQ$ для произвольных n. Осцилляторная волновая функция $\chi_n(Q)$ имеет вид

$$\chi_n(Q) = \sqrt[4]{\frac{\omega}{\pi}} \frac{1}{\sqrt{2^2 n!}} \exp\left(-\frac{1}{2}\omega Q^2\right) H_n(\sqrt{\omega}Q)$$

где H_n - полиномы Эрмита. Поэтому

$$C_n = \frac{\sqrt{\omega}}{\sqrt{\pi 2^n n1}} \int \exp\left[-\frac{1}{2}\omega Q^2 - \frac{1}{2}\omega(Q-\delta)^2\right] H_n(\sqrt{\omega}Q)dQ.$$

Этот интеграл легко вычислить, используя производящие функции полиномов Эрмита

$$\exp\left(-t^2 + 2t\xi\right) = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(\xi).$$

В результате получается

$$C_n = \frac{\alpha^n}{\sqrt{n!}} \exp\left(-\frac{1}{2}\alpha^2\right),$$

где $\alpha^2 = \frac{1}{4}\omega\delta^2 = \frac{2\pi}{\omega^3}(q\eta)^2$.

Вероятность испускания квантов с различными $k\lambda$ равна произведению квадратов выражений $C_n = \frac{\alpha^n}{\sqrt{n!}} \exp\left(-\frac{1}{2}\alpha^2\right)$, т. е.

$$W = \exp\left[-\sum_{k\lambda} \alpha_{k\lambda}^2\right] \prod_{k\lambda} \frac{\left(\alpha_{k\lambda}\right)^{2n} k\lambda}{(n_{k\lambda})!}.$$

Найдем среднее число квантов, излученных при торможении:

$$\bar{n}_{k\lambda} = \sum_{n_{k\lambda}} n_{k\lambda} w_n^{k\lambda} = \exp\left[-\alpha_{k\lambda}^2\right] \sum_{n_{k\lambda}} \frac{\left(\alpha_{k\lambda}\right)^{2n} k\lambda}{(n_{k\lambda})!} n_{k\lambda} =$$

$$= \exp\left[-\alpha_{k\lambda}^2\right] \sum_{n_{k\lambda}} \frac{\alpha_{k\lambda}^2}{(n_{k\lambda}-1)!} \left(\alpha_{k\lambda}\right)^2 \left(n_{k\lambda}^{-1}\right) = \alpha_{k\lambda}^2 = \frac{2\pi}{\omega_{k\lambda}^3} \left(q\eta_{k\lambda}\right)^2.$$

Таким образом, для вероятности испускания n квантов тина $\boldsymbol{k}, \lambda$ мы получаем следующую формулу:

$$w_n^{k\lambda} = \frac{\left(\bar{n}_{k\lambda}\right)^n k\lambda}{(n_{k\lambda})!} \exp\left(-\bar{n}_{k\lambda}\right).$$

Она совпадает с распределением Пуассона.

Вероятность испускания одного кванта данного типа, как видно из $w_n^{k\lambda} = \frac{(\bar{n}_{k\lambda})^n k\lambda}{(n_{k\lambda})!} \exp(-\bar{n}_{k\lambda})$, равна

$$\boldsymbol{w}_1^{k\lambda} = \bar{n}_{k\lambda} \exp(-\bar{n}_{k\lambda}).$$

При $\bar{n}_{k\lambda} \ll 1$ получаем $w_1^{k\lambda} \approx \bar{n}_{k\lambda}$. Это выражение совпадает с результатом обычной теории возмущений. (?????)

Из (2.68) мы видим, что сечение чисто упругого рассеяния строго равняется нулю. На опыте под упругим рассеянием понимают рассеяние, при котором энергия излученных квантов меньше некоторой величины E_1, которая определяется точностью измерения. Наблюдаемое сечение рассеяния равно

$$\sigma_{\text{набл}} = \sigma_0 W_0'.$$

Здесь σ_0 - вычисленное сечение упругого рассеяния без учета излучения, W_0' - вероятность того, что не излучено ни одного кванта с энергией, большей E_1. Как мы видели,

$$W_0' = \exp\left[-\int_{E_1}^{E} \frac{2\pi}{\omega^3} (q\eta_{k\lambda})^2 \frac{\omega^2 d\omega}{c^3(2\pi)^3}\right] = \exp\left[-2\pi \frac{2}{3} \frac{1}{(2\pi)^3} \frac{q^2}{c^3} \ln \frac{E}{E_1}\right].$$

В качестве верхнего предела мы взяли энергию электрона, хотя предположение о мягкости квантов нарушается уже при меньших энергиях. Если $\ln(E/E_1)$ достаточно велико, то это внесет малую ошибку.

Сечение излучения произвольного числа квантов любого типга равно

$$\sigma = \sigma_0 \sum_n W_n = \sigma_0$$

Если бы мы пользовались теорией возмущений, то получилось **b**

$$w_1^{k\lambda} = \frac{2\pi}{\omega_{k\lambda}^3} (q\eta_{k\lambda})^2,$$

$$W_1 = \sum_{k\lambda} w_1^{k\lambda} = \frac{2\pi \cdot 2q^2}{(2\pi)^3 c^3} \int_0^E \frac{d\omega}{\omega},$$

т.е. выражение, расходящееся на нижнем пределе. Эта расходимость, связанная с незаконным применением теории возмущений, называется инфракрасной расходимостью («инфракрасной катастрофой»).

(?!?!?? еще раз продумаю все это!!!!!)

6.7.9 Adiabatic Methods: Other Statements

Как догадаться про адиабатические методы?

(потом продумаю, пока есть просто предположения)

What if one takes into account "measurements" at the intermediate stage?

In adiabatics, we assume that change of the energy level is occurring after the evolution. Not like a particle can be measured ones it locates at a new level. This is the big question about measurement, and we are not touching it here. Change of the state in scope of the adiabatic

method happens only by change of coefficients and this is what we are dealing with. Thus it is only an approximate method for toy models and in real life, there are a lot of interactions in the intermediate dynamics which are not taken into account.

(???? but how to take into account that a particle can be measured at the intermediate stage of dynamics??? Maybe, it is related to Quantum Zeno effect?)

6.8 Variational methods: basics

6.8.1 Variational methods by Tong

(его читал, впишу, очень хорошее объяснение)

6.8.2 Variational methods by Zhou

(его читал, впишу, очень хорошее объяснение)

$$
\begin{aligned}
\Delta E= & \frac{8\pi^2 e^2}{4\pi\epsilon_0}\left(\frac{Z^3}{\pi a_0^3}\right)^2 \int dr_1 r_1^2 e^{-2Zr_1/a_0} \int dr_2 r_2^2 e^{-2Zr_2/a_0} \int\limits_{-1}^{+1} d\left(\cos\theta_2\right) \frac{1}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}} \\
= & -\frac{2\pi e^2}{\epsilon_0}\left(\frac{Z^3}{\pi a_0^3}\right)^2 \int dr_1 r_1^2 e^{-2Zr_1/a_0} \int dr_2 r_2^2 e^{-2Zr_2/a_0} \frac{\sqrt{\left(r_1-r_2\right)^2}-\sqrt{\left(r_1+r_2\right)^2}}{r_1r_2} \\
= & -\frac{2\pi e^2}{\epsilon_0}\left(\frac{Z^3}{\pi a_0^3}\right)^2 \int dr_1 r_1^2 e^{-2Zr_1/a_0} \int dr_2 r_2^2 e^{-2Zr_2/a_0} \frac{|r_1-r_2|-|r_1+r_2|}{r_1r_2} \\
= & \frac{8\pi e^2}{\epsilon_0}\left(\frac{Z^3}{\pi a_0^3}\right)^2 \int\limits_{r_2}^{\infty} dr_1 r_1 e^{-2Zr_1/a_0} \int\limits_0^{\infty} dr_2 r_2^2 e^{-2Zr_2/a_0} \\
= & \frac{8\pi e^2}{\epsilon_0}\left(\frac{Z^3}{\pi a_0^3}\right)^2 \int\limits_0^{\infty} dr_2 r_2^2 \left(\frac{a_0 r_2}{2Z}+\frac{a_0^2}{4Z^2}\right) e^{-4Zr_2/a_0} \\
= & \frac{5}{8}\frac{Ze^2}{4\pi\epsilon_0 a_0} = \frac{5Z}{4}Ry
\end{aligned}
$$

6.8.3 Variational proof that any 2D potential well supports at least one bound state by Yang, de Llano

(такое пока сам я не могу сделать, нужно будет - поучусь у них этому, небольшая статья)

6.9 Semiclassical methods

Обсудим подробно квазиклассику (или ВКБ методы, JWKB, WKB).

6.9.1 Main Semiclassical Methods

(по идее это в 1ю часть перенесу)

итоговые методы

вроде бы тут дело в том, что мы хотим научиться приближенно решать некоторые типичные диффуры в классических, то есть больших по сравнению с $\hbar$, масштабах.

(??)

Здесь волновая функция представлена как показательная функция, квазиклассически расширенная, а затем или амплитуда, или фаза медленно изменяются.

$$\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + U(x) = E \to S(x) = \int\limits_{x_0}^{x} p(x)dx, \quad p(x) = \sqrt{2m(E-U(x)}$$

Решения этого уравнения буквально соответствуют классическому действию как функции координат.

Однако, несложно Вычислить поток на такой волновой функции, мы получим $j(x) = \hbar p(x)/m$ - а в стационарных состояниях этот поток обязан не зависеть от координат.

Поэтому необходим учёт следующего порядка, который восстанавливает унитарность.

Тем самым, общий вид волновой функции в квазиклассическом приближении имеет вид (тут и дальше мы положили $\hbar = 1$):

$$\psi_{\pm}(x) = \frac{e^{\pm i\int\limits_{x_0}^{x} p(x)dx}}{\sqrt{p(x)}}, \quad \psi(x) = c_+\psi_+(x) + c_-\psi_-(x)$$

$$\psi_{\pm}(x) = \frac{c_{\pm}}{\sqrt{|p(x)|}} e^{\pm\int\limits_{x_0}^{x}|p(x)|dx}|, \quad |p(x)\,| = \sqrt{2m(U(x)-E)}$$

$$\left|\frac{dp}{dx}\right| \ll p^2 \leftrightarrow \left|\frac{d\lambda}{dx}\right| \ll 1 \leftrightarrow m\left|\frac{\partial U/\partial x}{p^3}\right| \ll 1$$

Алгоритм вывода правил Бора-Зоммерфельда (!?!?!??!)

(часто это нужно, я пока хз.)

сшивка

$$x < x_0 \to z < 0: \quad p(z) = \sqrt{-z}, \quad S(z) = \int\limits_0^z p(z)dz = -\frac{2}{3}(-z)^{3/2},$$

$$\psi_{\pm}(z) = \frac{1}{(-z)^{1/4}}\exp\left(\mp\frac{2}{3}i(-z)^{3/2}\right)$$

$$x > x_0 \to z > 0, \quad |p(z)| = \sqrt{z}, \quad \tilde{S}(z) = \int\limits_0^z |p(z)|dz = \frac{2}{3}z^{3/2}$$

$$\psi_{\pm}(z) = \frac{1}{z^{1/4}}\exp\left(\pm\frac{2}{3}z^{3/2}\right)$$

$$-\psi''(z) + z\psi(z) = 0 \to \psi(z) = C_1\,\mathrm{Ai}(z) + C_2\,\mathrm{Bi}(z)$$

$$\mathrm{Ai}(|z|\gg 1)\approx\begin{cases}\frac{1}{2\sqrt{\pi}z^{1/4}}\exp\left(-\frac{2}{3}z^{3/2}\right), & z>0,\\ \frac{1}{\sqrt{\pi}(-z)^{1/4}}\sin\left(\frac{2}{3}(-z)^{3/2}+\frac{\pi}{4}\right) & z<0\end{cases},$$

$$\mathrm{Bi}(|z|\gg 1)\approx\begin{cases}\frac{1}{\sqrt{\pi}z^{1/4}}\exp\left(\frac{2}{3}z^{3/2}\right), & z>0\\ \frac{1}{\sqrt{\pi}(-z)^{1/4}}\cos\left(\frac{2}{3}(-z)^{3/2}+\frac{\pi}{4}\right), & z<0\end{cases}$$

Метод WKB в комплексной плоскости (!?!)

(связь с компланом, да! тут еще линии Стокса, которые не шарю.)
(!!! в 1ю часть многое перенесу, важные, типичные темы!!!)

Преобразование уравнения Шредингера и классический его предел по Киселеву

Согласно принципу соответствия у квантовой системы должен существовать классический предел, в котором дисперсии физических величин малы при рассмотрении динамики их средних значений. Как мы отмечали, такой предел обычно имеет место при больших квантовых числах $n\to\infty$, когда дисперсией можно пренебречь. Принцип соответствия использовался при построении основных операторов физических величин в приближении геометрической оптики, которая как раз дает предельный случай волновой механики, когда пренебрежение эффектами интерференции позволяет говорить о траектории корпускул, составляющих свет.

Другой аспект принципа соответствия открывается, если взглянуть на соотношение неопределенностей физических наблюдаемых $\hat{A}$ и $\hat{B}$:

$$\Delta A\cdot\Delta B\geqslant\frac{\hbar}{2}|\langle\hat{C}\rangle|.$$

Можно считать, что флуктуации наблюдаемых малы, если

$$\hbar\to 0.$$

Кроме того, дискретность спектра физической величины, как мы видели, связана с конечностью значения постоянной Планка, так что этой дискретностью можно пренебречь, если верно (12.1). Конечно, это условие является лишь необходимым, но не достаточным (знак неравенства в соотношении неопределенностей). Тем не менее, исследование предела (12.1) позволяет установить и достаточные признаки применимости классического описания и приближений к нему.

Запишем волновую функцию как

$$\Psi(\boldsymbol{r},t)=A(\boldsymbol{r},t)\mathrm{e}^{\frac{i}{\hbar}S(\boldsymbol{r},t)},$$

где $A(\boldsymbol{r},t),S(\boldsymbol{r},t)\in\mathbb{R}$ т.е. в виде вещественной амплитуды A и фазы S.

Сперва вычислим

$$\Delta\Psi=\nabla^2\Psi=\boldsymbol{\nabla}\cdot\left\{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(\boldsymbol{r},t)}\boldsymbol{\nabla}A+\frac{\mathrm{i}}{\hbar}A\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(\boldsymbol{r},t)}\nabla S\right\}=$$
$$=\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(\boldsymbol{r},t)}\left\{2\frac{\mathrm{i}}{\hbar}\boldsymbol{\nabla}S\cdot\nabla A+\Delta A-\frac{1}{\hbar^2}A(\boldsymbol{\nabla}S)^2+\frac{\mathrm{i}}{\hbar}A\triangle S\right\},$$

и также

$$\frac{\partial}{\partial t}\Psi=\left\{\frac{\partial A}{\partial t}+\frac{\mathrm{i}}{\hbar}A\frac{\partial S}{\partial t}\right\}\mathrm{e}^{\frac{i}{\hbar}S(r,t)},$$

Подставим это в уравнение Шрёдингера $\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\triangle\Psi + V\Psi$, возьмем мнимую и вещественную части, находим

$$\hbar\frac{\partial A}{\partial t} = -\frac{\hbar}{2m}\{2\nabla S\cdot\nabla A + A\triangle S\}$$
$$-A\frac{\partial S}{\partial t} = -\frac{\hbar^2}{2m}\triangle A + \frac{A}{2m}(\nabla S)^2 + VA.$$

Запишем их в виде

$$\frac{\partial A}{\partial t} + \frac{1}{m}\nabla S\cdot\nabla A + \frac{A}{2m}\triangle S = 0,$$
$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V = \frac{\hbar^2}{2m}\frac{\triangle A}{A}$$

(ниже - в 1 часть дублирую!)

Найдем

$$j = -\frac{\mathrm{i}\hbar}{2m}\left\{\Psi^*\nabla\Psi - (\nabla\Psi)^*\Psi\right\} = \frac{A^2}{m}\nabla S$$

и

$$\operatorname{div} j = \nabla\cdot j = \frac{2}{m}A\nabla S\cdot\nabla A + \frac{A^2}{m}\triangle S.$$

Поэтому, домножая $\frac{\partial A}{\partial t} + \frac{1}{m}\nabla S\cdot\nabla A + \frac{A}{2m}\triangle S = 0$ на $2A$, получаем

$$2A\frac{\partial A}{\partial t} + \operatorname{div} j = 0$$

и с учетом того, что

$$\rho = |\Psi|^2 = A^2,$$

находим, что это уравнение сводится к уравнению непрерывности

$$\frac{\partial\rho}{\partial t} + \operatorname{div} j = 0.$$

(???? почему это не в самом начале, тривиальные вещи!!!)

Второе уравнение из уравнения Шредингера $\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V = \frac{\hbar^2}{2m}\frac{\triangle A}{A}$ при $\hbar\to 0$ сводится к уравнению Гамильтона-Якоби:

$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V = 0.$$

Как и следовало ожидать, мы пришли к классическому пределу уравнения Шрёдингера. При этом комплексная фаза волны $S/\hbar$ удовлетворяет принципу Ферма.

(?? почему???)

Для стационарного состояния $\frac{\partial\rho}{\partial t} = 0, \frac{\partial S}{\partial t} = -E$ имеем из $\frac{\partial A}{\partial t} + \frac{1}{m}\nabla S\cdot\nabla A + \frac{A}{2m}\triangle S = 0$ уравнение

$$(\nabla S)^2 - 2m(E-V) = \hbar^2\frac{\Delta A}{A}$$

вместе с уравнением нулевой дивергенции потока вероятности.

Классический импульс есть:

$$p^2 \equiv 2m(E-V) \equiv \left(\frac{\hbar}{\lambda}\right)^2.$$

(тоже укажу это лучше в 1 части)

Поэтому

$$(\nabla S)^2 = \frac{\hbar^2}{\lambda^2}\left(1 + \lambda^2 \frac{\Delta A}{A}\right).$$

Следовательно, классическое приближение применимо, если

$$\lambda^2 \frac{\Delta A}{A} \ll 1.$$

Тогда имеет место уравнение для волнового фронта в геометрической оптике:

$$(\nabla \Phi)^2 = \frac{1}{\lambda^2}, \quad \Phi = \frac{1}{\hbar} S.$$

(с ним в оптике нужно лучше разобраться!)

Метод JWKB по Киселеву

Метод JWKB состоит в решении уравнений из уравнения Шрёдингера

$$\frac{\partial A}{\partial t} + \frac{1}{m}\nabla S \cdot \nabla A + \frac{A}{2m}\triangle S = 0,$$
$$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V = \frac{\hbar^2}{2m}\frac{\triangle A}{A}$$

в виде рядов по $\hbar$.

Нулевое приближение

Первое для стационарных состояний есть

$$2S'A' + AS'' = 0,$$

где штрих означает дифференцирование по координате частицы x. Из него:

$$A(x) = \frac{C}{\sqrt{S'(x)}}.$$

Значит, амплитуда волновой функции однозначно (с точностью до нормировки C) задается ее фазой.

Второе уравнение

$$(\nabla S)^2 - 2m(E - V) = \hbar^2 \frac{\Delta A}{A}$$

решается с подстановкой $A(x) = \frac{C}{\sqrt{S'(x)}}$, при которой $A' = -\frac{S''}{2\sqrt{(S')^3}}$, $A'' = \frac{3(S'')^2}{4\sqrt{(S')^5}} - \frac{S'''}{2\sqrt{(S')^3}}$

Получим

$$(S')^2 - 2m(E - V) = \frac{\hbar^2}{4(S')^2}\left\{3(S'')^2 - 2S'S'''\right\}.$$

Отсюда следует, что фаза раскладывается в ряд по степеням $\hbar^2$:

$$S = S_0 + \hbar^2 S_2 + \hbar^4 S_4 + ...$$

Поскольку волновую функцию можно теперь записать как

$$\Psi(x) = \exp\left\{\frac{\mathrm{i}}{\hbar}S(x) + \ln A(x)\right\} = C\exp\left\{\frac{\mathrm{i}}{\hbar}S(x) - \frac{1}{2}\ln S'\right\}$$

ясно, что разложение фазы приводит и к разложению амплитуды по степеням $\hbar^2$, а вещественного аргумента экспоненты - по нечетным степеням $\hbar$.

(!! в 1ю часть укажу это тоже, типичные свойства!!!)

Решаем методом итераций. Нулевая итерация:

$$\{S_0'(x)\}^2 = p^2(x), \quad p^2 = 2m[E - V(x)],$$

причем необходимо выполнение условия вещественности фазы, так что $p^2(x) \geqslant 0, E \geqslant V(x)$.

Это значит, что пока нулевая итерация справедлива только в области, доступной для классической частицы. При этом

$$p(x) = \pm\sqrt{2m[E - V(x)]},$$

и возможно существование двух линейно независимых решений (в зависимости от значения энергии в согласии с общими свойствами решений одномерного уравнения Шрёдингера).

Решение уравнения имеет стандартный вид координатной части действия классической частицы:

$$S_0(x) = \int p \, \mathrm{d}x$$

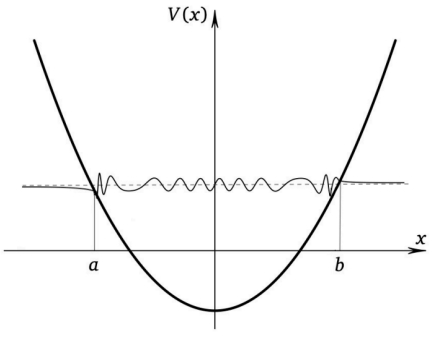
С учетом вклада энергии в комплексную фазу стационарного состояния

$$S_0(x,t) = \int p \, \mathrm{d}x - E \, \mathrm{d}t$$

получаем волновую функцию в классическом пределе

$$\Psi(x,t) = C \exp\left\{\frac{\mathrm{i}}{\hbar} S_0(x,t)\right\} = C \exp\left\{\frac{\mathrm{i}}{\hbar} \int p \, \mathrm{d}x - E \, \mathrm{d}t\right\}$$

В итоге фаза волновой функции осциллирует в области, доступной для классической частицы, например, между точками поворота, как показано на рис. 13.



Осциллирующее поведение волновой функции в этой области показано волнистой кривой, а в запрещенной для классического движения области пси-функция убывает экспоненциально. Продолжение в классически недоступную область. Заметим, что выведенная нами пара уравнений не изменится, если получать их, выделяя не мнимую и вещественную части в уравнении Шрёдингера, а вклады в виде четной и нечетной функций по $\hbar$.

В самом деле, считая, что A и S-четные функции по $\hbar$, опять приходим к (12.3) и (12.1). Значит, нулевая итерация в классически запрещенной области координаты дает решение в виде

$$\Psi(x) = C_1 \mathrm{e}^{+\frac{1}{r}} \int \sqrt{2m[V(x)-E]}\mathrm{d}x + C_2 \mathrm{e}^{-\frac{1}{r}} \int \sqrt{2m[V(x)-E]}\mathrm{d}x,$$

причем C_1, C_2 зависят от налагаемых на волновую функцию граничных условий.

Например, на рис. выше волновая функция должна экспоненциально убывать на бесконечности, так что поведение при $x \to +\infty$ требует $C_1 = 0$.

(?!?! выделю ключевые формулы потом, пока их так себе вижу.)

Квазиклассическое приближение

Учтем линейный по $\hbar$ вклад в аргумент экспоненты для волновой функции, т.е. подставим выражение для функции A через S_0. Тогда

$$\Psi(x) = \frac{C}{\sqrt{p(x)}} \exp\left\{\frac{\mathrm{i}}{\hbar}\int p(x)\mathrm{d}x\right\},$$

где импульс $p(x) = \sqrt{2m[E-V(x)]}$ уже комплекснозначная двулистная функция, т.е. имеется пара решений уравнений Шрёдингера в квазиклассическом приближении. При этом необходимо помнить, что граничные условия, а именно наличие классического финитного движения при заданной энергии, могут приводить к фиксированной суперпозиции этих решений, так как при финитном движении в одномерном случае состояние энергии невырождено.

Для первой итерации, дающей квадратичный по $\hbar$ вклад в S, имеем

$$\left(S_0' + \hbar^2 S_2'\right)^2 \approx p^2(x) + \frac{\hbar^2}{4\left(S_0'\right)^2}\left\{3\left(S_0''\right)^2 - 2S_0'S_0'''\right\}.$$

Поскольку с заданной точностью до $\hbar^2$

$$\left(S_0' + \hbar^2 S_2'\right)^2 \approx \left(S_0'\right)^2 + 2\hbar^2 S_0'S_2'$$

и $S_0' = p(x)$, получаем

$$S_2' = \frac{1}{8p^3}\left\{3\left(p'\right)^2 - 2pp''\right\}.$$

Условия применимости квазиклассики

Чтобы нулевая итерация для S_0 была хорошим приближением, необходимо выполнения условия $\hbar^2\left|S_2'\right| \ll \left|S_0'\right|$, то есть

$$\left|\frac{\hbar^2}{p^3}\left(p'\right)^2\right| \ll |p| \qquad \to \qquad \left|\frac{\hbar}{p}\frac{p'}{p}\right| \ll 1,$$
$$\left|\frac{\hbar^2}{p^3}p''p\right| \ll |p| \qquad \to \qquad \left|\frac{\hbar^2}{p^2}\frac{p''}{p}\right| \ll 1.$$

Величина

$$p'\frac{\hbar}{p} = p'\lambda\!\!\!^{-} = \delta p$$

есть изменение импульса на расстоянии в длину волны в первом порядке. Поэтому разложение по $\hbar$ оправдано, если

$$\left|\frac{\delta p}{p}\right| \ll 1,$$

т.е. если относительное изменение импульса на длине волны пренебрежимо мало в первом порядке.

Условие $\left|\frac{\hbar^2}{p^2}\frac{p''}{p}\right| \ll 1$ дает

$$\left|\frac{\delta^2 p}{p}\right| \ll 1, \quad \delta^2 p \sim p''\lambda\!\!\!^{-2},$$

т.е. относительное изменение импульса на длине волны должно быть пренебрежимо мало и во втором порядке.

С учетом

$$p = \frac{\hbar}{\lambda\!\!\!^{-}}, \quad \frac{p'}{p} = -\frac{\lambda\!\!\!^{-\prime}}{\lambda\!\!\!^{-}}$$

условия применимости квазиклассического приближения можно записать в виде

$$|\lambda\!\!\!^{-\prime}| \ll 1, \quad |\lambda\!\!\!^{-\prime\prime}\lambda\!\!\!^{-}| \ll 1,$$

что, по сути, означает, что относительное изменение длины волны на расстоянии в длину волны в первом и втором порядке должно быть пренебрежимо мало.

Условие $|\lambda\!\!\!^{-\prime}| \ll 1$ можно также переформулировать так: если ℓ - интервал, на котором потенциал изменяется настолько существенно, что изменение длины волны сравнимо с длиной волны, то

$$|\lambda\!\!\!^{-\prime}| \sim \frac{\lambda\!\!\!^{-}}{\ell}$$

откуда сразу находим

$$\frac{\lambda}{\ell} \ll 1,$$

а значит, существенное изменение потенциала в условиях применимости квазиклассики происходит на расстояниях ℓ, в которые укладывается большое число длин волн. Другими словами, потенциал должен изменяться достаточно медленно.

(?? еще раз потом посмотрю, почему именно медленно???? пока еще не разобрался.)

Кроме того, используя явный вид функции $p(x)$, запишем

$$p' = -\frac{2mV'}{2p} = \frac{m}{p}F,$$

где $F = -V'$ - сила, действующая на частицу. Тогда

$$\frac{\hbar}{p}F \approx \delta x \cdot F \sim \delta A$$

есть работа, совершаемая силой на расстоянии $\delta x = \hbar/p = \lambda$, т.е. на длине волны.

С учетом $T_{\text{kin}} = \frac{p^2}{2m}$, условие применимости квазиклассики в первом порядке принимает вид

$$\left|\frac{\delta A}{T_{\text{kin}}}\right| \ll 1,$$

т.е. работа, совершаемая силой на длине волны, должна быть пренебрежимо мала в сравнении с кинетической энергией частицы. Поэтому ясно, что вблизи точек поворота, где кинетическая энергия и импульс стремятся к нулю, а сила остается отличной от нуля, квазиклассическое приближение неприменимо.

Плотность потока вероятности в квазиклассике по Киселеву

Подставим в $j = -\frac{i\hbar}{2m}\left\{\psi^*\psi' - (\psi')^*\psi'\right\}$ выражение $\Psi_\pm(x) = \frac{C_\pm}{\sqrt{p(x)}}\exp\left\{\pm\frac{\mathrm{i}}{\hbar}\int\limits_{x_0}^{x} p(x)\mathrm{d}x\right\}$, у которой $\psi' = \frac{C_\pm}{\sqrt{p(x)}}\left(-\frac{1}{2}\frac{p'(x)}{p(x)} \pm \frac{\mathrm{i}}{\hbar}p(x)\right)\exp\left\{\pm\frac{\mathrm{i}}{\hbar}\int\limits_{x_0}^{x} p(x)\mathrm{d}x\right\} \approx \pm\frac{\mathrm{i}}{\hbar}p(x)\frac{C_\pm}{\sqrt{p(x)}}\exp\left\{\pm\frac{\mathrm{i}}{\hbar}\int\limits_{x_0}^{x} p(x)\mathrm{d}x\right\}$. Учтено, что согласно критерию применимости $\left|\frac{\hbar^2}{p^2}\frac{p''}{p}\right| \ll 1$, имеем $-\frac{1}{2}\frac{p'(x)}{p(x)} \pm \frac{\mathrm{i}}{\hbar}p(x) \approx \pm\frac{\mathrm{i}}{\hbar}p(x)$.

Получаем

$$j\left[\psi_\pm\right] \approx \pm\frac{|C_\pm|^2}{m}.$$

Это значит, что частица, которая согласно квазиклассическому приближению (12.25) имеет волновую функцию ψ_+, движется по направлению оси координат, а ψ_- - в обратном направлении.

Подчеркнем, что в выражение для потока вероятности в квазиклассическом приближении (12.26) формально уже не входит зависимость от импульса как функции координат: постоянные $C_\pm$ могут быть заданы из соображений, связанных с постановкой задачи.

Для сравнения, у свободной нерелятивистской частицы импульс $p(x) = p > 0$ не зависит от координат, так что квазиклассическое выражение для волновой функции (12.25) является точным, а постоянные $C_\pm$выбираются из соображений нормировки волны де Бройля так, что $C_\pm/\sqrt{p} = 1$, и тогда получается стандартный вывод, что поток вероятности свободной нерелятивистской частицы в волне де Бройля задается скоростью движения частицы.

(??? где нужна эта формула??)

Условия отражения, сшивка решений в точках поворота по Киселеву

Вблизи точек поворота вместо квазиклассического приближения необходимо точно решить уравнение Шрёдингера. Тогда

$$E - V(x) \approx E - V(a) - V'(a)(x-a) = F(a)(x-a),$$

где в точке поворота $V(a) = E$, и мы приходим к уравнению Шрёдингера для частицы, на которую действует постоянная сила $F(a)$. Точное решение выражается через спецфункцию Эйри, которую необходимо затем сшить с квазиклассическим приближением возле точки поворота. Результат такого строгого рассмотрения в точности согласуется с более наглядным методом сшивки квазиклассических решений вблизи точки поворота, который мы и приведем ниже. По сути, речь идет об отражении частицы от потенциального барьера в квазиклассическом приближении.

Пусть слева от точки поворота $x = a$ расположена недоступная для классической частицы область вплоть до $x \to -\infty$. Волновая функция при $x < a$ есть

$$\Psi(x) = \frac{C}{2}\frac{1}{\sqrt[4]{2mV'(a)(x-a)}}\exp\left\{\frac{1}{\hbar}\int\limits_{a}^{x}\sqrt{2mV'(a)(x-a)}\mathrm{d}x\right\},$$

где

$$V'(a) < 0,$$

так что аргументы корней положительны. Как функция комплексной переменной x выражение ((12.27) является четырехлистной функцией с разрезом, который начинается в точке поворота a и направлен по вещественной оси в сторону $x > a$. Арифметическое значение корней в формуле (12.27) в области, недоступной для классической частицы, отвечает выбранному граничному условию с затуханием волновой функции вглубь области, не доступной для частицы в рамках классической механики, $x < a$.

Покажем, что выражение (12.27) отвечает асимптотическому поведению волновой функции, которую возле точки поворота можно найти точно, решая стационарное уравнение Шрёдингера с линейным потенциалом

$$V(x) = E + V'(a)(x-a), \quad V(a) = E, \quad V'(a) < 0,$$

если перейти от точного решения в область, где становится применима квазиклассика. Уравнение Шрёдингера с линейным потенциалом (12.28)

$$\frac{\hat{p}^2}{2m}|\Psi\rangle + V(\hat{x})|\Psi\rangle = E|\Psi\rangle$$

можно записать в импульсном представлении для $\tilde{\Psi}(p) = \langle p|\Psi\rangle$, если ввести оператор

$$\hat{y} = \widehat{x-a} = \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}p},$$

откуда

$$\frac{p^2}{2m}\tilde{\Psi}(p) + V'(a)\mathrm{i}\hbar\frac{\mathrm{d}\bar{\Psi}(p)}{\mathrm{d}p} = 0.$$

Точное решение этого уравнения находится элементарно, так как

$$\frac{\mathrm{d}\bar{\Psi}}{\tilde{\Psi}t} = \frac{\mathrm{i}}{\hbar}\frac{p^2}{2mV'(n)}\mathrm{d}p \to \ln\tilde{\Psi} = \frac{\mathrm{i}}{\hbar}\frac{p^3}{6mV'(a)} + \text{ const.}$$

Значит,

$$\tilde{\Psi}(p) = \tilde{\Psi}_0 \exp\left\{\frac{i}{\hbar}\frac{p^3}{6mV'(a)}\right\}.$$

Поэтому волновую функцию в координатном представлении можно найти, взяв обратное преобразование Фурье,

$$\Psi(x) = \Psi_A(y)|_{y=x-a} = \tilde{\Psi}_0\int\frac{\mathrm{d}p}{2\pi\hbar}\exp\left\{\frac{\mathrm{i}}{\hbar}\left(yp + \frac{p^3}{6mV'(a)}\right)\right\}\Bigg|_{y=x-a}.$$

Иными словами,

$$\Psi(x) = \tilde{\Psi}_0\int\frac{\mathrm{d}p}{2\pi\hbar}\mathrm{e}^{\varphi(p)}, \quad \varphi(p) = \frac{\mathrm{i}}{\hbar}\left\{(x-a)p + \frac{p^3}{6mV'(a)}\right\}.$$

Вещественная специальная функция, заданная в (12.32), при условии затухания вглубь потенциального барьера называется функцией Эйри. Найдем экстремум функции $\varphi(p)$, вычислив производную

$$\varphi'(p) = \frac{\mathrm{i}}{\hbar}\left\{(x-a) + \frac{p^2}{2mV'(a)}\right\}.$$

Точка экстремума $p = p(x)$,

$$\frac{p(x)^2}{2m} = -V'(a)(x-a) = E - V(x),$$

расположена при $p^2(x) < 0$, если $x < a$. Поскольку

$$\varphi''(p) = \frac{\mathrm{i}}{\hbar}\frac{p}{mV'(a)},$$

получаем разложение функции $\varphi(p)$ возле точки экстремума $p(x)$ с точностью до членов второго порядка малости где $\varphi(p) = \varphi(p(x)) + \frac{1}{2}(p-p(x))^2\varphi''(p(x)) + \mathcal{O}\left((p-p(x))^3\right)$,

$$\begin{aligned}
&\varphi(p(x)) = \frac{\mathrm{i}}{\hbar}(x-a)p(x)\left\{1 + \frac{p^2(x)}{6mV'(a)(x-a)}\right\} = \\
&= \frac{\mathrm{i}}{\hbar}(x-a)p(x)\left\{1 - \frac{1}{3}\right\} = \frac{\mathrm{i}}{\hbar}(x-a)p(x) \\
&\text{a } \varphi''(p(x)) = \frac{\mathrm{i}}{\hbar}\frac{p(x)}{mV'(a)} = \frac{1}{\hbar}\frac{1}{mV'(a)}\sqrt{2mV'(a)(x-a)},
\end{aligned}$$

где мы выбрали значение

$$p(x) = -\mathrm{i}\sqrt{2mV'(a)(x-a)}, \quad x < a,$$

и поэтому

$$\varphi''(p(x)) < 0, \quad x < a.$$

Это значит, что в интеграле (12.32) при $x < a$ подынтегральное выражение ведет себя гауссовым образом, а поправки в разложении функции (12.34) приводят к малым поправкам к значению интеграла

$$\begin{aligned}
\int \frac{\mathrm{d}p}{2\pi\hbar}\mathrm{e}^{\varphi(p)} &\approx \mathrm{e}^{\varphi(p(x))}\int \frac{\mathrm{d}p}{2\pi\hbar}\exp\left\{\frac{1}{2}(p-p(x))^2\varphi''(p(x))\right\} = \\
&= \frac{1}{2\pi\hbar}\mathrm{e}^{\varphi(p(x))}\sqrt{-\frac{2\pi}{\varphi''(p(x))}} = \mathrm{e}^{\varphi(p(x))}\sqrt{\frac{mV'(a)}{2\pi\hbar}}\frac{1}{\sqrt[4]{2mV'(a)(x-a)}}
\end{aligned}$$

Заметим теперь, что с выбранным нами значением экстремальной точки (12.37) интеграл от импульса в точности совпадает с найденным нами выражением для значения функции $\varphi(p)$ в экстремальной точке (12.35),

$$\begin{aligned}
&\frac{1}{\hbar}\int_a^x \sqrt{2mV'(a)(x-a)}\mathrm{d}x = \frac{1}{\hbar}\sqrt{-2mV'(a)}\int_a^x (a-x)^{\frac{1}{2}}\,\mathrm{d}x = \\
&= -\frac{2}{3}\frac{1}{\hbar}\sqrt{-2mV'(a)}(a-x)^{\frac{3}{2}} = \frac{2}{3}(x-a)\sqrt{2mV'(a)(x-a)} = \\
&= \frac{i}{\hbar}(x-a)p(x)\frac{2}{3} = \varphi(p(x)).
\end{aligned}$$

Таким образом, мы показали, что вычисление асимптотики точного решения уравнения Шрёдингера с линейным потенциалом возле точки поворота воспроизводит волновую функцию квазиклассического приближения в области, где эта функция затухает вглубь потенциального барьера (12.27).

Интересно рассмотреть вопрос о поправке к полученной асимптотике. Для этого нужно вычислить третью производную

$$\varphi'''(p) = \frac{\mathrm{i}}{\hbar}\frac{1}{mV'(a)},$$

так что поправки в подынтегральном выражении могут быть представлены в виде ряда

$$\exp\left\{\frac{1}{3!}\varphi'''(p(x))(p-p(x))^3\right\} = 1 + \left\{\frac{1}{3!}\varphi'''(p(x))(p-p(x))^3\right\} + \\ + \frac{1}{2!}\left\{\frac{1}{3!}\varphi'''(p(x))(p-p(x))^3\right\}^2 + \ldots$$

Значит, гауссов интеграл приобретает поправки в виде

$$\int \mathrm{d}p \mathrm{e}^{\phi(p)} = \mathrm{e}^{\phi(p(x))} \int \mathrm{d}p \exp\left\{-\frac{1}{2}\frac{(p-p(x))^2}{\delta p^2}\right\} \times \\ \times \left(1 + \left\{\frac{1}{3!}\varphi'''(p(x))(p-p(x))^3\right\} + \frac{1}{2!}\left\{\frac{1}{3!}\varphi'''(p(x))(p-p(x))^3\right\}^2 + \ldots\right) = \\ = \mathrm{e}^{\phi(p(x))} \int \mathrm{d}p \exp\left\{-\frac{1}{2}\frac{(p-p(x))^2}{\delta p^2}\right\} \left(1 + \frac{1}{2!}\left\{\frac{1}{3!}\varphi'''(p(x))(p-p(x))^3\right\}^2 + \ldots\right),$$

где мы исключили нулевой вклад от третьей степени по импульсу, так как нечетные степени в гауссовом интеграле обращаются в нуль в силу свертки четной функции с нечетной. Вклад шестой степени легко найти, если заметить, что гауссов интеграл

$$\int \mathrm{d}p \exp\left\{-\frac{1}{2}\frac{(p-p(x))^2}{\delta p^2}\right\} = \sqrt{2\pi\delta p^2}$$

а

$$\int \mathrm{d}p \exp\left\{-\frac{1}{2}\frac{(p-p(x))^2}{\delta p^2}\right\} (p-p(x))^2 = \delta p^2 \sqrt{2\pi\delta p^2},$$

и это дисперсия гауссова распределения, умноженная на нормировочный множитель. Значит,

$$\int \mathrm{d}p \exp\left\{-\frac{1}{2}\frac{(p-p(x))^2}{\delta p^2}\right\} (p-p(x))^6 = \\ = 2^2 \frac{\partial}{\partial 1/\delta p^2}\frac{\partial}{\partial 1/\delta p^2} \int \mathrm{d}p \exp\left\{-\frac{1}{2}\frac{(p-p(x))^2}{\delta p^2}\right\} (p-p(x))^2 = \\ = 4\frac{\partial}{\partial 1/\delta p^2}\frac{\theta}{\partial 1/\delta p^2}\left(\delta p^2\sqrt{2\pi\delta p^2}\right) = 15\left(\delta p^2\right)^3\sqrt{2\pi\delta p^2}.$$

Поэтому

$$\int \mathrm{d}p \mathrm{e}^{\phi(p)} \approx \mathrm{e}^{\phi(p(x))}\sqrt{2\pi\delta p^2}\left\{1 + \frac{1}{2!}\left\{\frac{1}{3!}\varphi'''(p(x))\right\}^2 15\left(\delta p^2\right)^3\right\}.$$

В этом выражении

$$\delta p^2 = -\frac{1}{\varphi''(p(x))} = -\left(\frac{\mathrm{i}}{\hbar}\frac{p(x)}{mV'(a)}\right)^{-1} = -\hbar m V'(a)\frac{1}{\sqrt{2mV'(a)(x-a)}},$$

как это и необходимо для квазиклассического выражения для волновой функции

$$\Psi(x) = \frac{C}{\sqrt{p(x)}}\exp\left\{\frac{1}{\hbar}\int\limits_a^x |p(x)|\mathrm{d}x\right\}$$

а подстановка $\varphi'''(p(x))$ из (12.38) приводит к поправке в виде

$$\Psi(x) \mapsto \Psi(x)\left(1+\frac{5}{24}\frac{1}{\hbar^2}mV'(a)\left(\frac{\hbar}{\sqrt{2mV'(a)(x-a)}}\right)^3\right) = \\ = \Psi(x)\left(1+\frac{5}{24}\frac{\hbar}{|p(x)|}V'(a)\frac{1}{|p^2(x)|/m}\right).$$

Из этого выражения видно, что безразмерная поправка к волновой функции казиклассического приближения имеет следующий порядок по постоянной Планка с чертой $\hbar$. Эта поправка мала в области применимости квазиклассики, так как определяется отношением работы сил на длине волны к кинетической энергии,

$$\left|\frac{\hbar}{|p(x)|}V'(a)\frac{1}{|p^2(x)|/m}\right| \sim \left|\lambda F\frac{1}{T_{\text{kin}}}\right| \sim \left|\frac{\delta A}{T_{\text{kin}}}\right| \ll 1.$$

Таким образом, мы убедились, что вычисление асимптотики точного решения уравнения Шрёдингера с линейным потенциалом согласуется с квазикласическим приближением и методом JWKB с вычислением рядов по $\hbar$.

Совершенно ясно, что теперь нужно найти асимптотическое поведение точного решения уравнения Шрёдингера с линейным потенциалом возле точки поворота перед потенциальным барьером при $x > a$. В этой области условие на экстремум (12.33) имеет два решения на разных берегах разреза в комплексной плоскости импульса: напомним, что разрез направлен по оси x от $x = a$, т.е. от точки поворота в сторону от барьера в область, доступную для частицы в классической механике.

Теперь, во-первых, интеграл будет вычисляться как сумма двух вкладов в экстремальных точках,

во-вторых, вместо гауссова интеграла возникнут интегралы возле стационарных точек комплексной фазы, так как выражения для функции $\varphi(p)$ и ее второй производной в экстремальной точке: (12.35) и (12.36), - становятся чисто мнимыми.

И наконец, в-третьих, нет никакой нужды повторять проведенные нами для случая гауссова интеграла выкладки, поскольку асимптотика интегралов со стационарной фазой вычисляется аналитическим продолжением результатов, полученных для гауссовых интегралов! Значит, нужно вычислить аналитическое продолжение выражения (12.27) на 2 берега разреза в комплексной области импульса и сложить два этих вклада в волновую функцию в координатном представлении, так как интеграл есть сумма ведущих вкладов, в данном случае, вкладов возле точек стационарной фазы. Совершпм переход в классически доступную область $x > a$ по двум контурам в комплексной плоскости x, как показано на рис. 14, так, чтобы оставаться вдали от точки поворота в области применимости квазиклассического приближения. Рис. 14. Контуры обхода точки поворота Для этого сделаем замену переменных

$$x - a = -\rho e^{i\phi}, \quad \rho = \text{ const } > 0,$$

где для контура с отрицательной мнимой частью координаты

$$0 \leqslant \phi \leqslant \pi$$

а для контура с положительной мнимой частью координаты

$$0 \geqslant \phi \geqslant -\pi$$

При таком обходе точки поворота с помощью аналитического продолжения (12.27) соответственно получаем пару вкладов при $x > a$

$$\Psi_1(x) = \frac{C}{2}\frac{\mathrm{e}^{-1\pi/4}}{\sqrt{p(x)}}\exp\left\{\frac{\mathrm{i}}{\hbar}\int\limits_a^x p(x)\mathrm{d}x\right\}$$
$$\Psi_2(x) = \frac{C}{2}\frac{\mathrm{e}^{\mathrm{i}\pi/4}}{\sqrt{p(x)}}\exp\left\{-\frac{\mathrm{i}}{\hbar}\int\limits_a^x p(x)\mathrm{d}x\right\}$$

где уже

$$p(x) = \sqrt{2\pi n\,(-V'(a)\rho)} = \sqrt{2m[E - V(x)]}, \quad x > a, \quad E > V(x),$$

- вещественная функция импульса. Решения $\Psi_{1,2}(x)$ представляют собой пару линейно независимых квазиклассических решений в области, доступной для классической частицы, которые мы уже заранее знаем в общем виде с точностью до комплексных констант в предэкспоненияльных множителях. Но

теперь рассмотренная нами процедура обхода точки поворота по контурам рис. 14, исходя из заданного вида (12.27), позволила однозначно определить связь предэкспоненциальных множителей с исходной константой C в формуле (12.27). Два контура отвечают переходу к разным берегам разреза, который идет от точки поворота a вдоль луча $x > a$. В квантовой механике берется суперпозиция этих двух линейно независимых решений. Поскольку задача одномерная и волновая функция обращается в нуль при $x \to -\infty$, спектр является невырожденным, и при вещественном значении константы C в формуле (12.27) вещественная при $x < a$ волновая функция будет вещественной и при $x > a$. Это требование при $x > a$ дает решение $\Psi_1(x) + \Psi_2(x)$, которое согласуется с описанным обходом точки поворота в комплексной плоскости, либо $\mathrm{i}\ \Psi_1(x) - \mathrm{i}\Psi_2(x)$, которое не согласуется с асимптотическим поведением точного решения уравнения Шрёдингера волизи точки поворота при условии затухания волновой функции вглубь потенциального барьера. Другими словами, мы не только знаем, что решение в классически доступной области будет вещественным, а из точного решения возле точки поворота мы знаем и модуль амплитуды этого решения, и фазы, которые в области применимости квазиклассики однозначно дают $\Psi_1(x) + \Psi_2(x)$, исходя из метода нахождения асимттотического поведения интеграла Фурье способом аналитического продолжения из области гауссова перевала к точкам стационарной фазы. В итоге

$$\Psi(x)_{x>a} = \Psi_1(x) + \Psi_2(x) = \frac{C}{\sqrt{p(x)}}\cos\left\{\frac{1}{\hbar}\int\limits_a^x p(x)\mathrm{d}x - \frac{\pi}{4}\right\}.$$

Таким образом, поскольку волны Ψ_2 и Ψ_1 в (12.42) и (12.41) можно соответственно рассматривать как падающую на потенциальный барьер волну и отраженную от него волну (см. раздел 12.3 и формулу для потока вероятности (12.26)), при отражении от классически недоступной области потенциала возникает относительная фаза волн $^1\frac{\pi}{2}$. Точнее, отраженная от потенциального барера волна отстает по фазе на $\frac{\pi}{2}$ от падающей на потенциальный барьер волны. И этот вывод не зависит от того, как расположен барьер, справа или слева от области, доступной для частицы в классической механике. Важно лишь, что в глубине потенциального барьера у потенциала нет сингулярных точек.

Совершенно аналогично при отражении от потенциального барьера справа при $x = b$

затухающая волновая функция в классически недоступной области

$$\Psi(x)_{x>b} = \frac{C}{2}\frac{1}{\sqrt{|p(x)|}}\exp\left\{\frac{1}{\hbar}\int\limits_x^b |p(x)|\mathrm{d}x\right\}$$

переходит в

$$\Psi(x)_{x<b} = \frac{C}{\sqrt{p(x)}}\cos\left\{\frac{1}{\hbar}\int\limits_x^b p(x)\mathrm{d}x - \frac{\pi}{4}\right\}.$$

Снова убеждаемся, что фаза падающей на потенциальный барьер волны на $\frac{\pi}{2}$ больше фазы отраженной волны.

Подчеркнем для примера сингулярного поведения потенциала, что в случае отражения от бесконечно высокого в точке поворота, непроницаемого потенциального барьера конечной ширины волновая функция должна обращаться в нуль в точке поворота, так что, например, если $V(x<a) = +\infty$, ТО

$$\Psi(x)_{x>a} = \frac{C}{\sqrt{p(x)}}\cos\left\{\frac{1}{\hbar}\int\limits_a^x p(x)\mathrm{d}x \pm \frac{\pi}{2}\right\}$$

и относительная фаза падающей и отраженной волн равна $\pm\pi$, т.е. вдвое болыше, чем в случае потенциального барьера конечной высоты в точках поворота, отличных от бесконечности. Подчеркнем, что в случае бесконечно высокого непроницаемого барьера импульс $p(x)$ отличен от нуля бесконечно близко к точке поворота a, так что $p(a+0) = p_0 > 0$, так что квазиклассикой можно воспользоваться вплоть до самой точки поворота, если, конечно, при $x > a$ выполняется критерий применимости квазиклассики, т.е. потенциал и, следовательно, импульс меняются достаточно медленно на длине волны, и установить вполне обоснованно условие $\Psi(a+0) = 0$, которое приводит к (12.46)

Правило квантования Бора–Зоммерфельда по Киселеву

Рассмотрим параболическую потенциальную яму, изображенную на рис. 13. Согласно полученным нами условиям сшивки решения внутри ямы с затухающими на бесконечности решениями получаем

$$\Psi(x)_{x>a} = \frac{C}{\sqrt{p(x)}}\cos\left\{\frac{1}{\hbar}\int\limits_a^x p(x)\mathrm{d}x - \frac{\pi}{4}\right\}$$

Н

$$\Psi(x)_{x<b} = \frac{\tilde{C}}{\sqrt{p(x)}}\cos\left\{\frac{1}{\hbar}\int\limits_x^b p(x)\mathrm{d}x - \frac{\pi}{4}\right\},$$

где C и $\tilde{C}$ - пормировотные копстапты для решспий, затухающих соответственно при $x \to \mp\infty$. Эти выражения должны быть тождественно равны друг другу, так как они описывают волновую функцию внутри классически доступной для частицы области. Значит,

$$\frac{C}{\sqrt{p(x)}}\cos\left\{\frac{1}{\hbar}\int\limits_a^x p(x)\mathrm{d}x - \frac{\pi}{4}\right\} = \frac{\tilde{C}}{\sqrt{p(x)}}\cos\left\{\frac{1}{\hbar}\int\limits_x^b p(x)\mathrm{d}x - \frac{\pi}{4}\right\}.$$

Это равенство имеет место, если, во-первых, амплитуды косинусов равны по модулю:

$$|C| = |\tilde{C}|,$$

а во-вторых, зависящие от координат фазы косинусов совпадают с точностью до знака и сдвига на πn:

$$\frac{1}{\hbar}\int_a^x p(x)\mathrm{d}x - \frac{\pi}{4} = \pm\left\{\frac{1}{\hbar}\int_x^b p(x)\mathrm{d}x - \frac{\pi}{4}\right\} + \pi n, \quad n \in \mathbb{Z}.$$

Знак «плюс» дает

$$\frac{1}{\hbar}\int_a^x p(x)\mathrm{d}x + \frac{1}{\hbar}\int_b^x p(x)\mathrm{d}x = \pi n,$$

так что слева стоит функция от x, а справа - постоянная: это уравнение не имеет решений ($p(x) \equiv 0$ не имеет физического смысла). Взяв знак «минус», находим

$$\frac{1}{\hbar}\int_a^b p(x)\mathrm{d}x = \pi\left(n + \frac{1}{2}\right).$$

Здесь интеграл берется по полупериоду движения классической частицы в потенциальной яме. Переходя к интегрированию по полному периоду, находим правило квантования Бора-Зоммерфельда:

$$\oint p(x)\mathrm{d}x = 2\pi\hbar\left(n + \frac{1}{2}\right), \quad n \in \{0 \cup \mathbb{N}\}.$$

Интеграл по циклу есть не что иное, как адиабатический инвариант фазовый объем внутри траектории. Поэтому квазиклассическое квантование связанных состояний частицы показывает, что квантовое число n задает число ячеек фазового пространства $\Delta\Gamma = 2\pi\hbar$, приходящихся на данное стационарное состояние (с точностью до вклада основного состояния). Ясно, что фазовый объем равен целому числу ячеек только при некоторых дискретных значениях энергии частицы.

Поскольку критерием применимости квазиклассического приближения является условие медленного изменения потенциала, это означает, что между точками поворота в потенциальной яме должно укладываться большое количество длин волн, т.е. число колебаний n в формуле (12.65) должно

быть много большим единицы: $n \gg 1$. Тогда возникает естественный вопрос о превышении точности, так как

Однако добавка одной второй имеет следующий смысл: при вычислении следующего порядка по $\hbar^2$ в методе JWKB поправка может оказаться сравнимой с вкладом $\frac{1}{2}$ в ведущем приближении, так что выражение в правой части (12.65) вполне правомерно и просто необходимо в рамках заданного порядка по.

Об обобщениях (????)

Отметим также, что в потенциалах общего вида правая часть (12.65) может принимать другое значение:

$$2\pi\hbar\left(n + \frac{1}{2}\right) \mapsto 2\pi\hbar\left(n + \gamma_M\right),$$

где γ_M носит имя «индекс Маслова».

При выводе $\gamma_M = \frac{1}{2}$ мы предполагали, что волновая функция вне области, доступной для классической частицы плавно убывает до нуля на бесконечности. Однако это становится неверно, если имеется, например, непроницаемый потенциальный барьер, расположенный на конечном расстоянии от потенциальной ямы, или сам потенциал сингулярен в конечном числе точек с ограниченными координатами. Тогда наше предположение о характере убывания волновой функции вне потенциальной ямы может оказаться неверным, и индекс Маслова принимает значение, отличное от $\frac{1}{2}$. К примеру, радиальное движение в центральном потенциале с учетом вклада центробежных сил отвечает случаю, когда и эффективный потенциал сингулярен как $1/r^2$, и движение ограничено областью $r \geqslant 0$. Поэтому квазиклассическое приближение для радиального движения в центральном потенциале существенно корректируется за счет индекса Маслова: это станет ясно при рассмотрении задачи рассеяния.

В более общем случае, когда у потенциала есть несколько потенциальных ям и потенциальных бареров условие квантования Бора-Зоммерфельда легко вывести, используя метод transfer-matrix, который мы подробно описали в параграфе на стр. 209. Ясно также, что рассмотренный нами вывод в случае одной потенциальной ямы и двух точек поворота вполне согласуется с методом transfer-matrix, а индекс Маслова для сингулярных потенциалов легко вводится в матрицу фазовых сдвигов (12.55) в соответствующих точках поворота.

Плотность состояний по Киселеву

Продифференцируем формулу квантования Бора-Зоммерфельда по энергии

$$\oint \frac{\partial p}{\partial E}\, \mathrm{d}x = 2\pi\hbar \frac{\partial n}{\partial E}.$$

Здесь, очевидно, $\frac{\partial n}{\partial E}$ - плотность спектра состояний по энергии, а $\frac{\partial E}{\partial p} = v$ - скорость движения частицы. Так как $\mathrm{d}x = v\, \mathrm{d}t$, интеграл по периоду сводится к

$$\oint \frac{\mathrm{d}x}{v(x)} = \oint \mathrm{d}t = T,$$

т.е. он равен периоду движения классической частицы. Отсюда

$$\frac{\partial E}{\partial n} = \frac{2\pi\hbar}{T} = \hbar\omega,$$

и плотность состояний определяется круговой частотой движения $\omega = 2\pi/T$. Эта частота не зависит от энергии у гармонического осциллятора, так что квазиклассика воспроизводит точный результат для разности энергий между двумя соседними уровнями:

$$\Delta E = \frac{\partial E}{\partial n}\Delta n\bigg|_{\Delta n=1} = \hbar\omega.$$

В произвольном потенциале частота движения и расщепление между уровнями связанных состояний зависят от энергии.

Нормировка

При нормировке волновой функции связанного состояния в квазиклассическом приближении необходимо учесть два факта: 1) плотность вероятности обнаружить частицу вне классически доступной области пренебрежимо мала (экспоненциально

подавлена); 2) само приближение справедливо лишь при $n \gg 1$, т.е. когда число волн между точками поворота велико (в противном случае длина волны заведомо сильно изменялась бы за период колебаний от бесконечности в точке поворота до конечного значения внутри допустимого интервала координат). Значит,

$$\int\limits_{-\infty}^{+\infty} |\Psi(x)|^2 \, \mathrm{d}x \approx \int\limits_{a}^{b} |\Psi(x)|^2 \, \mathrm{d}x = |C|^2 \int\limits_{a}^{b} |\cos\{\cdot\}|^2 \frac{\mathrm{d}x}{p(x)}.$$

Здесь под косинусом стоит фаза, которая совершает большое количество колебаний n, а амплитуда этих колебаний, обратно пропорциональная импульсу, по условию применимости квазиклассики медленно меняется. Значит, квадрат косинуса можно заменить его средним за период колебания:

$$\cos^2\{\cdot\} \to \frac{1}{2}.$$

Тогда с учетом $\mathrm{d}x = v \, \mathrm{d}t$ и $p = mv$ нормировка

$$\int\limits_{-\infty}^{+\infty} |\Psi(x)|^2 \, \mathrm{d}x \approx \frac{|C|^2}{2m} \int\limits_{a}^{b} \mathrm{d}t = \frac{|C|^2}{4m} T,$$

где опять T - полный период движения частицы в связанном состоянии. Волновая функция нормирована на единичную вероятность, так что

$$|C|^2 = \frac{4m}{T}.$$

Возмущение (!?!??!??!)

(!!! вроде это самое главное, потому что на эти формулы и решаются задачи!!!)

Рассмотрим задачу квазиклассического квантования связанных состояний системы с гамильтонианом

$$\hat{H} = \frac{\hat{p}^2}{2m} + V_0(x) + \delta V(x)$$

с малым возмущением $\delta V \ll V_0$ в смысле малого отличия интегралов от функций V_0 и $V_0 + \delta V$ на разумных конечных интервалах координаты. Будем считать, что решение задачи с гамильтонианом

$$\hat{H}_0 = \frac{\hat{r}^2}{2m} + V_0(x)$$

известно, так чтп

$$\oint p_0^E(x) \mathrm{d}x = 2\pi\hbar \left(n + \frac{1}{2}\right),$$

где, естественно,

$$p_0^E(x) = \sqrt{2m\,[E_n - V_0(x)]},$$

и интеграл берется между точками поворота (a, b). В задаче с возмущением правило квантования Бора-Зоммерфельда дает

$$\oint p^{E+\delta E}(x) \mathrm{d}x = 2\pi\hbar \left(n + \frac{1}{2}\right),$$

где импульс

$$p^{E+\delta E}(x) = \sqrt{2m\,[E_n + \delta E_n - V_0(x) - \delta V(x)]}.$$

Здесь $E_n + \delta E_n = \tilde{E}_n$ - значение уровня энергии в потенциале с возмущением, и мы полагаем, что δE - малая поправка. Пределы интегрирования, конечно, несколько меняются: $(a + \delta a, b + \delta b)$, - но вклад вблизи точек поворота в квазиклассике пренебрежимо мал, так что в (12.73) и (12.75) мы будем полагать пределы интегрирования одинаковыми (в рамках ведущего приближения это оправдаНО).

Вычтем (12.73) из (12.75) при фиксированном n. Тогда имеем

$$\oint \left\{ p^{E+\delta E}(x) - p_0^E(x) \right\} \mathrm{d}x = 0.$$

Выражение для импульса можно разложить по малому возмущению энергии и потенциала:

$$\begin{aligned} p^{E+\delta E}(x) &= \sqrt{2m\left[E_n + \delta E_n - V_0(x) - \delta V(x)\right]} = \\ &= \sqrt{2m\left[E_n - V_0(x)\right]\left\{1 + \frac{\delta E_n - \delta V}{E_n - V_0(x)}\right\}} \approx p_0 + \frac{m}{p_0}\left[\delta E_n - \delta V\right]. \end{aligned}$$

Значит,

$$\delta E_n \oint \frac{\mathrm{d}x}{p_0} = \oint \frac{\mathrm{d}x}{p_0} \delta V(x)$$

Переходя к интегралу по времени, находим

$$\delta E_n = \frac{1}{T} \int\limits_0^T \mathrm{d}t \delta V[x(t)],$$

или

$$\delta E_n = \frac{m}{T} \oint \frac{\mathrm{d}x}{p_0(x)} \delta V(x).$$

Первая из этих формул показывает, что среднее значение возмущения за период определяет сдвиг энергии связанного состояния, а вторая дает практический рецепт расчета этого сдвига.

Критерий применимости квазиклассики

Проведенное рассмотрение расчета поправки к энергии стационарного состояния за счет возмущения в квазиклассическом приближении следует считать справедливым только в том случае, если, прежде всего, изменение волновой функции $\delta\psi$ в задаче с возмущением в некотором смысле мало по сравнению с самой волновой функцией ψ_0 в исходной задаче: $|\delta\psi| = |\psi - \psi_0| \ll |\psi_0|$. Так, потребуем, чтобы в ходе временнОй эволюции, выраженной в волновой функции фактором $\exp\{-\mathrm{i}Et/\hbar\}$, за время периода колебаний частицы в потенциальной яме T была мала поправка к волновой функции за счет разности энергий:

$$\left| \mathrm{e}^{-\frac{1}{\hbar}ET} - \mathrm{e}^{-\frac{1}{\hbar}E_0 T} \right| \ll 1 \leftrightarrow \left| \mathrm{e}^{-\frac{1}{\hbar}\delta E \cdot T} - 1 \right| \ll 1.$$

Последнее возможно, только если фаза под знаком экспоненты мала по сравнению с 2π, т.е. [1]

$$\left| \frac{\delta E \cdot T}{\hbar} \right| \ll 2\pi \leftrightarrow |\delta E| \ll \hbar\omega,$$

где стандартным образом фазовая частота $\omega = 2\pi/T$. Как мы показали, величина поправки к энергии определяется средним значением возмущения на классической

траектории с энергией уровня в системе без возмущения: $\delta E = \langle \delta V \rangle$, в то время как $\hbar\omega$ задает инкремент в дискретном спектре энергий системы ΔE. Поэтому критерий применимости теории возмущений в квазиклассическом случае (12.81) можно записать в виде

$$|\langle \delta V \rangle| \ll |\Delta E|.$$

Таким образом, теория возмущений применима при условии малости возмущения по сравнению с разностью энергий между соседними стационарными уровнями.

При выводе критерия применимости методом рассмотрения временного фактора волновой функции мы по сути полагали, что в некоторой точке

пространства в области, доступной для классической частицы и удаленной от точек поворота, где квазиклассика заведомо неприменима, пространственные волновые функции в задаче с возмущением и без возмущения практически совпадают, что и позволило рассмотреть лишь разность временных факторов. Но для этого необходимо, чтобы и пространственная зависимость этих волновых функция мало отличалась друг от друга. Поэтому запишем более подробно вид координатной зависимости волновой функции в квазиклассике, используя разложение импульса по малым поправкам при наличии возмущения:

$$\exp\left\{\frac{\mathrm{i}}{\hbar}\int p(x)\mathrm{d}x\right\} \simeq \exp\left\{\frac{\mathrm{i}}{\hbar}\int p_0(x)\mathrm{d}x\right\}\exp\left\{\frac{\mathrm{i}m}{\hbar}\int \frac{\mathrm{d}x}{p_0(x)}(\delta E - \delta V(x))\right\}.$$

Как мы уже установили, переход к временной зависимости на траектории дает

$$m\int\limits_{t_0}^{t}\frac{\mathrm{d}x}{p_0(x)} = t - t_0, \quad m\int\limits_{t_0}^{t}\delta V(x)\frac{\mathrm{d}x}{p_0(x)} = \langle \delta V(t)\rangle \cdot (t - t_0)\,,$$

где, конечно, время на верхнем пределе интегрирования параметрически зависит от координаты, $t = t(x)$. Значит, координатная зависимость волновой функции в задаче с возмущением может быть представлена в виде

$$\psi(x) = \psi_0(x)\exp\left\{\frac{\mathrm{i}}{\hbar}\delta E\cdot(t-t_0) - \frac{\mathrm{i}}{\hbar}\langle\delta V(t)\rangle\cdot(t-t_0)\right\},$$

причем первое слагаемое под знаком экспоненты по сути повторяет поправку во временном факторе за счет малого сдвига энергии стационарного состояния, и мы знаем, что возникающей за счет него фазой за период колебаний можно пренебречь. Поэтому критерий применимости теории возмущений, учитывающий малое отличие пространственной зависимости волновой функции в задаче с возмущением от зависимости исходной волновой функции, можно представить в виде

$$|\psi(x) - \psi_0(x)| \ll |\psi_0(x)| \leftrightarrow \left|\mathrm{e}^{\hbar\langle\delta V(t)\rangle\cdot(t-t_0)} - 1\right| \ll 1,$$

что опять же справедливо, только если на всем периоде колебаний набегающая фаза мала по сравнению с 2π, т.е.

$$\left|\frac{\langle\delta V(T)\rangle\cdot T}{\hbar}\right| \ll 2\pi \leftrightarrow |\langle\delta V\rangle| \ll |\Delta E| = \hbar\omega.$$

В итоге и рассмотрение пространственной зависимости волновых функций приводит к тому же критерию теории возмущений в квазиклассике: характерные значения возмущения на интервале классического движения частицы должны быть существенно меньше разности энергий между соседними уровнями. При этом не следует, конечно,

забывать и о критерии применимости самого квазиклассического приближения, а именно об условии большого числа колебаний за период движения между точками поворота: $n \gg 1$.

Еще более наглядно критерий применимости теории возмущений в квазиклассике можно представить, если определить при больших квантовых числах малую вариацию номера уровня δn:

$$\delta E_n = \frac{\mathrm{d}E_n}{\mathrm{d}n}\delta n,$$

где $\mathrm{d}E_n/\mathrm{d}n$ - обратная плотность состояний в спектре энергии, посредством которой расстояние между двумя соседними уровнями можно вычислить как

$$\Delta E = \frac{\mathrm{d}E_n}{\mathrm{d}n}\Delta n \quad \text{при } \Delta n = 1.$$

Тогда условие применимости теории возмущений $\Delta E \gg |\delta E_n|$ представится в виде

$$|\delta n| \ll 1,$$

т.е. возмущение эффективно сводится к малому сдвигу номера квантового состояния в задаче без возмущения, так что не происходит перекрытия с соседними уровнями.

Случаи применимости.

(Киселев даже для черных дыр видел применение, напишу потом.)
(??? даже для эл поз пар!!!! жесть вообще.)

Как догадаться про квазиклассику?

(this is a important question for understanding this topic, I'll think about it later))

5. Введение в квазиклассические методы или "старая квантовая механика" по Тахтаджаяну

Представленная выше формулировка квантовой механики восходит к 1925 - 1927-м годам и принадлежит Гейзенбергу, Шрёдингеру, Борну, Йордану и Дираку. Она заменила старую квантовую теорию, предложенную Бором в 1913-м году, базировавшуюся на планетарной модели атома Резерфорда. В старой теории уровни энергии одномерной квантовой системы соответствуют замкнутым орбитам ассоциированной классической гамильтоновой системы, удовлетворяющим правилу квантования Бора-Вильсона-Зоммерфельда (правилу БВЗ):

$$\oint p dq = 2\pi\hbar\left(n + \frac{1}{2}\right)$$

где n - неотрицательное целое число, и интегрирование ведется по замкнутой орбите в фазовом пространстве $\mathbb{R}^2$. Правила квантования Бора-Вильсона - Зоммерфельда применяются и к вполне интегрируемым гамильтоновым системам с несколькими степенями свободы (см. раздел 1.2.6 главы 1). А именно: пусть $F_1 = H_\mathrm{c}, ..., F_N - N$ независимых интегралов движения в инволюции. Правила квантования БВЗ - это

$$\oint_\gamma \boldsymbol{p} d\boldsymbol{q} = 2\pi\hbar\left(n_\gamma + \frac{1}{4}\,\mathrm{ind}\,\gamma\right),$$

где интегрирование ведется по всем 1-циклам γ в лагранжевом подмногообразии $\Lambda = \{(\boldsymbol{p},\boldsymbol{q}) \in \mathbb{R}^{2N} : H_\mathrm{c}(\boldsymbol{p},\boldsymbol{q}) = E, F_2(\boldsymbol{p},\boldsymbol{q}) = E_2, ..., F_{\boldsymbol{N}}(\boldsymbol{p},\boldsymbol{q}) = \ = E_N\}$, $\mathrm{ind}\ \gamma \in \mathbb{Z}$ - так

называемый индекс Маслова цикла γ в Λ. В одномерном случае замкнутая орбита - топологически круг, и ее индекс Маслова равен 2. В разделе 3.6.3 главы 3 будет показано, что, вообще говоря, правила квантования Бора-Вильсона - Зоммерфельда дают только асимптотику уровней энергии при $\hbar \to 0$. Однако для интегрируемых систем с дополнительной симметрией, таких как гармонический осциллятор или задача Кеплера, правила квантования БВЗ определяют уровни энергии точно. Мы покажем это в следующем разделе для гармонического осциллятора и в разделе 3.5.1 главы 3 для задачи Кеплера.

6.9.2 Tunneling Through a Barrier

(all about it here)

Model of a tunneling

(write that well-known theory, it should be already written on some of the pages)

Special cases of a tunneling

Tunnelling of a composite particle in presence of a magnetic field

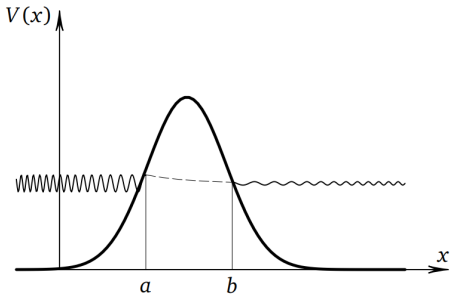
(there is an article with such a title. I'll learn it later, currently, I don't know how to describe it?)

6.9.3 Typical Examples and Details of the Semiclassical Method

(тут для задач особенности и задротские мелочи.)

Потенциальный барьер квазиклассикой

Рассмотрим задачу, в которой на потенциальный барьер с конечной силой возврата в точках поворота для классической частицы ограниченной энергии, т.е. фактически конечной высоты на конечном отрезке координат, в интервале $a < x < b$ слева падает и отражается волна. В этом случае экспоненциальное затухание волны в классически недоступной области потенциального барьера приводит к конечной, отличной от нуля волновой функции и в области $x > b$, где появляется уходящая на бесконечность волна, прошедшая через барьер (см. рис. 17).



Волновая функция

$$\Psi(x)_{x>b} - \frac{C}{\sqrt{p(x)}} \exp\left\{\frac{\mathrm{i}}{\hbar}\int_b^x p(x)\mathrm{d}x\right\}$$

имеет асимптотику прошедшей через барьер волны с потоком, направленным в положительном направлении x. Пользуясь методом сшивки решений в квазиклассическом приближении, описанным в предыдущем разделе, мы получим в области $a < x < b$ суперпозицию экспоненциально падающего и растущего с ростом x вкладов. Оба вклада нормированы так, чтобы при

обходе в комплексной плоскости точки поворота $x = b$ предэкспоненциальный множитель был бы задан одной и той же константой C в (12.87). Значит, в области $a < x < b$ возле $x = a$ в рамках погрешности самого квазиклассического приближения следует пренебречь тем вкладом, который экспоненциально подавлен, так как его учет означал бы превышение точности метода расчета. Поэтому, делая подстановку $p(x) \mapsto \mathrm{i}|p(x)|$, находим

$$\Psi(x)_{a<x<b} = \frac{C}{\sqrt{|p(x)|}} \mathrm{e}^{-\mathrm{i}\pi/4} \exp\left\{ -\frac{1}{\hbar} \int\limits_b^x |p(x)| \mathrm{d}x \right\} =$$

$$= \frac{C}{\sqrt{|p(x)|}} \mathrm{e}^{-\mathrm{i}\pi/4} \exp\left\{ -\frac{1}{\hbar} \int\limits_a^x |p(x)| \mathrm{d}x + \frac{1}{\hbar} \int\limits_a^b |p(x)| \mathrm{d}x \right\} \to$$

$$\to \quad \Psi(x)_{a<x<b} = \frac{\tilde{C}}{\sqrt{|p(x)|}} \exp\left\{ \frac{1}{\hbar} \int\limits_x^a |p(x)| \mathrm{d}x \right\},$$

$$\text{где } \tilde{C} = C \mathrm{e}^{-\mathrm{i}\pi/4} \exp\left\{ \frac{1}{\hbar} \int\limits_a^b |p(x)| \mathrm{d}x \right\}.$$

Эта волновая функция повторяет ситуацию, которая отвечает отражению волны от потенциального барьера, который находится справа от области, доступной для классической частицы при $x = a$, с затуханием волновой функции вглубь потенциального барьера, так что волновая функция слева от барьера должна вести себя как

$$\Psi(x)_{x<a} = \frac{\bar{C}}{\sqrt{p(x)}} 2 \cos\left\{ \frac{1}{\hbar} \int\limits_x^a p(x) \mathrm{d}x - \frac{\pi}{4} \right\}.$$

Коэффициент прохождения потенциального барьера $\mathcal{T}$ определяется отношением потоков вероятности в прошедшей и падающей волнах:

$$j_{\text{out}} = j_{x>b} = \frac{|C|^2}{p} \frac{p}{m} = \frac{|C|^2}{m},$$

и здесь при вычислении потока в волне дифференцируется только экспонента, а предэкспоненциальный множитель в квазиклассике изменяется очень медленно, т.е. выносится из-под знака дифференцирования, а после представления косинуса в области $x < a$ в виде суммы двух экспонент с падающей и отраженной волнами, получаем

$$j_{\text{in}} = \frac{|\tilde{C}|^2}{m},$$

так ЧТО [1]

$$\mathcal{T} = \left| \frac{C}{\tilde{C}} \right|^2 = \exp\left\{ -\frac{2}{\hbar} \int\limits_a^b |p(x)| \mathrm{d}x \right\}.$$

Отметим, что в квазиклассике коэффициент отражения тождественно равен единице (разложение косинуса на две экспоненты с одинаковыми амплитудами). Это не противоречит наличию ненулевого коэффициента прохождения, так как он экспоненциально подавлен, так что в разности $1-\mathcal{T}$ сохранение второго члена являлось бы превышением точности. Экспоненциальное подавление обусловлено условием достаточной ширины барьера, так как ширина должна превосходить несколько длин волн для применимости квазиклассики вдали от точек поворота:

$$\frac{1}{\hbar}\int\limits_a^b |p(x)|\mathrm{d}x \gg \pi \leftrightarrow \int\limits_a^b \frac{\mathrm{d}x}{\lambda} \gg \pi \to \frac{b-a}{\lambda} = \frac{\ell}{\lambda} \gg 1$$

где $\ell = b-a$ - характерная длина, на которой потенциал существенно изменился, что находится в согласии с общим условием применимости квазиклассики: длина волны существенно меняется на расстояниях, много больших длины волны, $\lambda/\ell \ll 1$.

Строго говоря, при выводе коэффициента прохождения потенциального барьера, т.е. при рассмотрении эффекта туннелирования, для применимости квазиклассического приближения необходимо, чтобы потенциал достаточно плавно вел себя вблизи точек поворота, так что, например, для потенциала на рис. 18 в области $0 < x < a$ нужно уже использовать точное решение уравнения Шрёдингера. Это, однако, сказывается только на предэкспоненциальном множителе в коэффициенте прохождения (12.89), который становится отличным от единицы [2]. Поэтому по-прежнему

$$\mathcal{T} \sim \exp\left\{-\frac{2}{\hbar}\int\limits_a^b |p(x)|\mathrm{d}x\right\}.$$

Туннельный эффект был использован Гамовым для объяснения закономерностей α-распада квазистационарных состояний ядер в соответствии с расчетом коэффициента прохождения в потенциале типа рис. 18, где притяжение (яма) обусловлено короткодействующими ядерными силами, а отталкивание-кулоновским взаимодействием положительного ядра и α-частицы.

Рис. 18.

Квазистационарное состояние в потенциальной яме и проникновение волны через потенциальный барьер В этой связи заметим, что квазистационарными состояниями называют долгоживущие резонансы, возникающие в процессах рассеяния, о которых мы упоминали в лекции 5. К теории рассеяния и распадам квазистационарных состояний мы обратимся несколько позднее во второй части курса. Здесь же укажем на то, что резонансы могут образовываться как при упругом рассеянии, когда начальное и конечное состояния описываются одним и тем же набором частиц, так и при неупругом, когда набор частиц изменяется. Долгое время жизни резонанса позволяет рассматривать его безотносительно к процессу его происхождения, а задачи описания квазистационарных состояний составляют отдельный класс, который мы не рассматриваем в этом курсе.

Флуктуации и виртуальные частицы

Физический смысл туннельного эффекта становится более ясным, если ввести понятие виртуальных частиц. В области потенциальной энергии, недоступной для классических частиц, имеют место существенные флуктуации, обусловленные тем, что операторы кинетической и потенциальной энергии по отдельности не коммутируют с

гамильтонианом:

$$[T(\boldsymbol{p}),\hat{H}]=\left[\frac{\boldsymbol{p}^2}{2m},V(\boldsymbol{r})\right]=\frac{1}{2m}(\boldsymbol{p}[\boldsymbol{p},V(\boldsymbol{r})]+[\boldsymbol{p},V(\boldsymbol{r})]\boldsymbol{p})=$$
$$=-\frac{\hbar^2}{2m}\Delta V(\boldsymbol{r})-\frac{\mathrm{i}\hbar}{m}\{\boldsymbol{\nabla}V(\boldsymbol{r})\}\cdot\boldsymbol{p}$$

и $[V(\boldsymbol{r}),\hat{H}]=-[T(\boldsymbol{p}),\hat{H}]\neq 0$, так что значения кинетической и потенциальной энергии имеют неопределенности в случае стационарного состояния с точно заданной энергией.

Этими флуктуациями можно пренебречь в области, доступной для классической частицы, потому что $-\nabla V=\boldsymbol{F}$ - сила, действующая на частицу, и второе слагаемое в коммутаторе (12.90) имеет порядок

$$\frac{\hbar}{m}\{\nabla V(\boldsymbol{r})\}\cdot\boldsymbol{p}\simeq\frac{\hbar Fp}{m}\sim F\cdot\frac{\hbar}{p}\frac{p^2}{m}\sim\delta A\cdot T_{\mathrm{kin}}\,,$$

где, как и выше, δA - работа силы на длине волны. Эта работа совершается за характерное время

$$\delta t\sim\frac{\lambda}{v}\sim\frac{\hbar}{p}\cdot\frac{m}{p}\sim\frac{\hbar}{T_{\mathrm{kin}}}.$$

Первое слагаемое в коммутаторе (12.90) также связано с работой на длине волны, если учесть поправку к значению силы на длине волны $\delta F\sim F'\lambda$,

$$-\frac{\hbar^2}{2m}\Delta V=\frac{\hbar^2}{2m}\nabla\cdot\boldsymbol{F}\simeq\frac{p^2}{2m}\frac{\hbar^2}{p^2}F'\sim T_{\mathrm{kin}}\,(\lambda\delta F)\sim T_{\mathrm{kin}}\,\delta' A.$$

Поскольку коммутатор с гамильтонианом определяет производную оператора по времени, для флуктуаций за время δt(12.91) находим

$$\mathrm{i}\hbar\frac{\delta T_{\mathrm{kin}}}{\delta t}\sim[T,\hat{H}]\to T_{\mathrm{kin}}\ \cdot\delta T_{\mathrm{kin}}\ \sim\delta A\cdot T_{\mathrm{kin}}\,,$$

а значит, согласно условию применимости квазиклассического приближения

$$\frac{\delta T_{\mathrm{kin}}}{T_{\mathrm{kin}}}\sim\frac{\delta A}{T_{\mathrm{kin}}}\ll 1,$$

и флуктуациями как кинетической, так и потенциальной энергии в классически доступной области необходимо пренебречь. Поэтому можно проводить рассуждения в терминах импульса, зависящего от потенциальной энергии, как мы это делали при построении квазиклассического приближения.

Ситуация коренным образом меняется в области, недоступной для классической частицы, когда понятия кинетической и потенциальной энергии плохо определены по отдельности. Итак, имеется вероятность такой флуктуации потенциальной энергии, при которой частица может проникнуть в классически недоступную область с некоторым положительным значением кинетической энергии. Эта вероятность в квазиклассике определяется коэффициентом прохождения

$$w\sim\mathrm{e}^{-2\frac{S}{\hbar}},$$

где S - действие, зависящее от координаты частицы в глубине потенциального барьера. Частицы, проникающие под барьер за счет флуктуаций потенциальной и кинетической энергии, называют виртуалвными. Таким образом, при наличии внешнего поля его потенциал испытывает флуктуации, приводящие κ распространению виртуальных

частиц. Если внешнее поле меняется, скажем, адиабатически в зависимости от времени или расстояния, то виртуальные частицы могут попасть в классически доступную область, т.е. наблюдаться, как это имеет место при прохождении через потенциальный барьер: если потенциал медленно уменьшается ниже значения полной энергии в некоторой области пространства, то в ней наблюдается туннельный эффект - виртуальные частицы за счет флуктуаций проходят барьер и регистрируются в классически доступной области как реальные.

Метод квазиклассики как способ учета возмущений (!?!?)

(важно обсудить это, если это применять, то по идее метод будет равносилен теории возмущений!)

Связь квазиклассики и теории возмущений (!??!?!!?)

(вопрос: как связаны эти два метода??? и как имея решение одним методом переписать его другим методом? пока слабо связь вижу, там - разложения, тут - приближенное решение. хз пока что.)

6.9.4 Semiclassical Approximation by MK (??)

В этой главе мы рассмотрим в одномерном и трехмерном случаях приближенный метод решения волнового уравнения, когда потенциал медленно изменяется на длине волны частицы. С простейшим случаем такого приближения мы познакомились в 1.1.

Одномерная задача

Напишем уравнение Шрсдингера в виде

$$\varphi'' + k^2(x)\varphi = 0$$

где

$$k^2(x) = 2[E - V(x)].$$

(считаем $\hbar = M = 1$). Пусть потенциил $V(x)$ достаточно медленно меняется с изменением координаты, так что

$$kl \geqslant 1,$$

где l - длина, на которой существенно меняется $V(x)$.

Тогда можно найти приближенное решение (3.1). Ишем решение (3.1) в виде $\varphi = Ae^{is}$, где A и S-действительные функции координаты. Имеем $\varphi' = e^{iS}\left(A' + iS'^2A\right)$ и $\varphi'' = e^{iS}\left(A'' + 2iS'A' + iS''A - S'^2A\right)$. Из (3.1) имеем

$$A'' + 2iA'S' - iS''A - S'^2A + k^2A = 0.$$

Отделяя вещественную часть от мнимой, получаем два соотношения:

$$A'' + S'^2A + k^2A = 0$$
$$S''A + 2A'S' = 0$$

Перепиинем
Отсюца (3.4)
в виде $\frac{A'}{A} = -\frac{S''}{2S'}$.

$$A = \frac{a}{\sqrt{S'}},$$

где a - постоянная величина. 13 (3.3) имеем

$$(S')^2 = k^2 + \frac{A''}{A}.$$

Так как k меняется суицественно на длине l, то и S', а следовательно, и A меняются существенно на той же длине. Поэтому $A''/A \sim 1/l^2$, т. е. $A''/k^2A \sim 1/(kl)^2 < 1$, и в первом приближении можно считать $(S')^2 = k^2$.

Тогда решение задачи имеет вид

$$\varphi(x) = \frac{a}{\sqrt{r}(x)} \exp\left[-i \int\limits_{x_1}^{x} k dx\right].$$

Это относится к случаю $E > V$, когда k вещественно. В случас $E < V$ решение будет содержать растущую и затухающую экспоненты, т. е.

$$\varphi(x) = A \exp\left[\pm \int\limits_{x_2}^{x} |k| dx\right],$$

где $A = a/\sqrt{|k|}$. Мы получили первое приближение в разложении по степеням величины $1/(kl)^2$. Ясно, как получать и следуюиие приближения. Оказывается, что получаюнийся при этом ряд по степеням параметра $1/(kl)^2$ асимптотический, а не обычный.

3 а ача. Показать, что при приближенной оценке производной от квазиклассической функции нужно дифференцировать лиив эксионенту.

Асимптотические ряды

Напомним, что такое асимнтотический ряд. Пусть

$$s_n = \sum_{v=0}^{n} \frac{a_\nu}{z^\nu}$$

- тастичная сумма ряла. Пусть при фиксированном z и $n \longrightarrow \infty$ величина $s_n \longrightarrow \infty$, но при фиксированном n и $z \longrightarrow \infty$ сумма s_n все лучшее и лучше аптроксимирует некоторую функцию $f(z)$, т. є.

$$\lim_{z\to\infty} z^n \left[s_n(z) - f(z)\right] = 0$$

Тогда говорят, что s_n есть асимптотическое представление $f(z)$. Это не есть ряд в обычном смысле этого слова, так как s_n расходится. Но из него можно извлечь сведения о функции $f(z)$, так как при $z \longrightarrow \infty$ он хорошо представляет эту функцию.

Построим $s_n(z)$ по заданноЙ $f(z)$. Величина s_0 равна a_0, следовательно, $a_0 = f(\infty)$. Величина $s_1 = a_0 + a_1/z$, тогда

$$\lim_{z\to\infty} z\left(a_0 + \frac{a_1}{z} - f(z)\right) = 0,$$

Т. е.

$$a_1 = \lim_{z\to\infty} z\,[f(z) - a_0] = \lim_{z\to\infty} z[f(z) - f(\infty)].$$

Аналогичным образом находятся все коэффициенты a_n.

Однако восстановить обратно функцию по ее асимптотическому представлению нельзя. Например, пусть $f(z) = e^{-z}$, тогда

$$a_0 = 0, \quad a_1 = \lim_{z\to\infty} ze^{-z} = 0, \quad a_2 = a_3 = ... = a_n = 0.$$

Следовательно, весь асимптотический ряд равен нулю для функции e^{-z}. Итак, функции $f(z)$ и $f(z) + e^{-z}$ имеют одиінаковые асимптотические представления.

Обозначим $z \equiv (kl)^2$. Оказывается, что квазиклассическое решение

$$\varphi_{\text{квазнкл}}\,(x) \approx \sum_{\nu=0}^{n} \frac{a_\nu(x)}{z^\nu}$$

есть асимптотический ряд, т. е. расходящийся при $n \to \infty$. Однако при $z \longrightarrow \infty$ величина $a_0(x)$ сколь угодно хорошо представляет функцию $\varphi(x)$ (точное решение).

Пусть, далее, z фиксировано. При $n \longrightarrow \infty$ ряд (3.6) расходится. Следовательно, при любом z есть оптимальное число членов $n(z)$, которое наилучшим образом описывает функцию $\varphi(x)$. Мы будем пользоваться только нулевым членом этого ряда. Следующие приближения не обязательно должны улучшить, они могут и ухудшить решение.

Поскольку квазиклассическое приближение есть асимптотический ряд по степеням параметра $1/(kl)^2$, в нем теряются эффекты, экспоненциально малые при больших значениях этого параметра.

Сиивание квазиклассических функций

В этом разделе мы найдем, как нужно сшивать квазиклассическую волновую функцию φ в области, доступной для классического движения, с φ в запреценной области. Для определенности предположим, что потенциальная энергия частицы имеет вид, изображенный на рис. 24 (начало координат взято в точке, где $V(x) = E$).

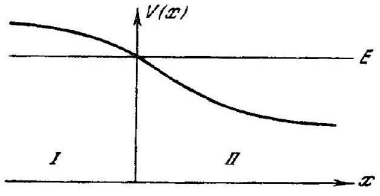


Рис. 24.

Квазиклассическое решение в области II (классически цоступной) согласно (3.5) имеет вид

$$\varphi = \frac{a_1}{\sqrt{k}} \exp\left(i\int_0^x k dx\right) + \frac{a_2}{\sqrt{k}} \exp\left(-i\int_0^x k dx\right),$$

а в области I (классически недостуінон)

$$\varphi = \frac{b_1}{\sqrt{|k|}} \exp\left(\int_x^0 |k| dx\right) + \frac{b_2}{\sqrt{|k|}} \exp\left(-\int_x^0 |k| dx\right)$$

Если бы квазиклассическое решение было аналитическо й функиий x в окрестности $x = 0$, то для нахождения соотношений между a_1, a_2 и b_1, b_2 нужно было бы аналитически продолжить это рсшение нз II в I (при этом экспоненты в (3.7) просто перешли бы в эксионенты (3.8)).

Правда, по вещественной оси нельзя было бы двигаться, так как в окрестности $x = 0$ квазиклассика негриленима ($k(0) = 0$, поэтому условие $kl \geqslant 1$ не вынолняется). Эту трудность можно было бы преодолеть, обойдя точку $x = 0$ в комнлексной плоскости по дуге достаточно большого радиуса (где применима квазиклассика).

Однако такое аналитическое продолжение дает, как мы увидим, неправильный результат.

Оказывается, что при таком обходе обязательно пере секаются линии (они называются линиями Стокса), где портится аналитическое продолжение. Поэтому такой способ нужно применять осторожно. Ниже мы покажем, как это сделать.

Дрругой возможный путь состоит в том, чтобы искать точное решение задачи вблизи $x = 0$, считая потенциал прямолинейным. Это решенне описывается так называемой функцией Эйри. Затем нужно сшить точное решение с квазиклассическим при $x > 0$ и $x < 0$.

Разумеется, так можно поступать только зная, что квазиклассическое піриближение становится применимым на расстояниях от точки поворота, малых по сравнению с расстоянием, на котором потенциал существенно отклоняется от прямолинейного. Покажем, что при большом параметре квазиклассичности ($k^2l^2 \gg 1$) это действительно так.

Разложим для этого потенциал $V(x)$ вблизи $x = 0$ в ряд: $V(x) \approx E + V'(0)x$. Тогда импульс $k(x) = \sqrt{-2V'(0)x} \equiv \alpha\sqrt{x}$. Оценим величину α : $\alpha \sim \sqrt{|V'(0)|} \sim \sqrt{\frac{V(0)}{l}} \sim \frac{k_0}{g}$, где $k_0 = \sqrt{2E}$, а l - длина, на которой существенно меняется потенциал $V(x)$. Итак, в окрестности точки $x = 0$ величина $k(x) \sim k_0\sqrt{\frac{x}{l}}$. Чтобы квазиклассическое приближение было применимо, нужно отони от точки $x = 0$ на такое расстояние, чтобы $d\left(\frac{1}{k}\right)/dx \ll 1$ или $\frac{\sqrt{l}}{k_0\sqrt{x^3}} \ll 1$. Отсюда находим: $x \gg l/\left(k_0 l\right)^{2/3}$. Так как $k_0 l \gg 1$, то можно выбрать такое x_1, Что

$$\frac{l}{\left(k_0 l\right)^{2/s}} \leqslant x_1 \ll l.$$

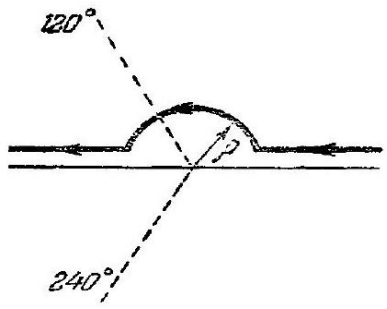
На расстояниях $\sim x_1$, с одной стороны, уже годится квазиклассическое приближение, а с другой, - нотенциал все еще можно считать прямолинейным.

Сшивка с помощью функций Эйри для потенциала, изображенного нар рис. 24, имеет вид)

$$\frac{1}{\sqrt{k}}\exp\left[i\int\limits_0^x k dx - \frac{\pi}{4}\right] \to \frac{1}{i\sqrt{|k|}}\exp\left[\int\limits_x^0 |h|dx\right] + \frac{1}{2\sqrt{|k|}}\exp\left[-\int\limits_x^0 |h|dx\right],$$

$$\frac{1}{\sqrt{k}}\exp\left[-i\int\limits_0^x k dx + \frac{\pi}{4}\right] \to \frac{-1}{i\sqrt{|k|}}\exp\left[\int\limits_x^0 |k|dx\right] + \frac{1}{2\sqrt{|k|}}\overline{|xp}\left[-\int\limits_x^0 |k|dx\right]$$

Сейчас мы получнм эти соотнонения, не прибегая к рункциям Эйрг. Выберем радиус обхода ρ порядка x_1 (рис. 25).



Тогда можно пользоваться квазнклассическим приближением и в то же время считать потенциал прямолинейным. Татк как при этом $k(x) = \alpha x^{1/2}$, то $\int\limits_0^x /2dx = \frac{2}{3}\alpha x^3/$В комплексной плоскости $x = \rho e^{i\varphi}$ и Prc. 25. $\int\limits_0^x k dx = \frac{2}{3}\alpha\rho^{3/2}\exp\left(\frac{3}{2}i\rho\right)$.

Поэтому

$\frac{1}{\sqrt{i2}}\exp\left[i\int\limits_0^i k dx\right] = \frac{1}{\sqrt{\alpha\omega^2/2}}e^{-i\frac{\varphi}{4}}\exp\left[\frac{2}{3}\alpha\rho^{3/2}\left(i\cos\frac{3}{2}\varphi - \sin\frac{3}{2}\varphi\right)\right]$

По mepe обхода контура Lo тех пор, пока $\varphi < \frac{2\pi}{3}$, $\sin\frac{3}{2}\varphi$ полоинтелен, а выражение (3.10) содержит затухающую экспоненту. Если $\varphi > \frac{2\pi}{3}$, то (3.10) содержит растущую экспоненту. Как только появпяется растущая эксионеита, все слагаемые, содержаиие убывающую экспоненту, не допжнь! учитываться, поскольку квазиклассическое приблужение, будучн аснмптотическим представлением, имеет по параметру квазнклассичности степенныio $\left(\sim\frac{1}{k^2l^2}\right)$, а не экспоненциальную точность.

При движении по окружности радиуса ρ в верхней по$i\frac{2}{3}\alpha x^3/2$

луплоскости выражение e переходит сначала в убывающщю экспоненту, а затем после пересечеция линии $\varphi = \frac{2\pi}{3}$ - в растущую экспоненту; как только появнлась растуцая экспонента, из-за неточности квазиклассического приближения возникает экспоненциально малая ошибка. Поэтому аналнтическоепродолжение позволяет найти коэфд-. фициент только при растуцей экспоненте.

Получанм

$$\frac{1}{\sqrt{k}}\exp\left[i\int\limits_0^x \dot{k}dx - \frac{\pi}{4}\right] \to \frac{1}{i\sqrt{|k|}}\exp\left[\int\limits_x^0 |k|dx\right].$$

При этом мы потеряли слагаемое, экспонениіально малое Ilo сравнению с правой частью (3.11).

При обходе точки $x = 0$ снизу функция (3.11) переходит сначала в растуцую эксионенту, а затем после пересечения линин

$$\mathscr{Q} = -\frac{2\pi}{3}$$

в убъвающчюо.

Iотерянная из-занеточности квазнклассического приближения в области $-\frac{2\pi}{3} < \varphi < 0$ экспоненциально malая добавка после перехода в область $-\pi < \varphi < -\frac{2\pi}{3}$ превращается в экспоненциально большой член, которьй такин образом теряется. Следовательно, такнм путем мы не можем получить правильное значение коэффициента при убывающей экспоненте. Как его получить? Предположим, что в классически недоступной области (при $V > E$ есть только затухающая экспонента:

$$\frac{1}{\sqrt{|k|}}\exp\left[-\int\limits_x^0 |k|dx\right]$$

Общее решение при $V < E$ имеет вид.

$$\frac{C_1}{\sqrt{\tilde{k}}}\exp\left[i\int\limits_0^x kdx - i\varphi_1\right] + \frac{C_2}{\sqrt{k}}\exp\left[-i\int\limits_0^x kdx + i\varphi_2\right]$$

Найдем C_1, C_2 и φ_1, φ_2. Для этого продіолжим аналитически (3.12) в область $x > 0$. Аналитическое продолжение через верхнюю полуплоскость имеет вид

$$\frac{1}{\sqrt{|k|}}\exp\left[-\int\limits_x^0 |k|dx\right] \to$$
$$\longrightarrow \frac{\exp[i\pi/4]}{\sqrt{\alpha\rho^{1/2}\exp(i\varphi/2)}}\exp\left[\frac{2}{3}\alpha\rho^{1/2}\left(\sin\frac{3}{2}\varphi - i\cos\frac{3}{2}\varphi\right)\right].$$

При $\varphi = 0$ получаем второе слагаемое (3.13), причем $\varphi_2 = -\pi/4, C_2 = 1$. Аналитически продолжая через нижнюю полуплоскость, мы получили бы первое слагаемое (3.13) со значениями

$$\varphi_1 = \varphi_2 = -\pi/4$$
$$C_1 = C_2 = 1$$

Каждый раз второе слагаемое теряется из-за экспоненциально малой ошибки в той области, где функция экспоненциально велика. Таким образом, имеем

$$\frac{1}{\sqrt{|k|}}\exp\left[-\int\limits_x^0 |k|dx\right] \to \frac{2}{\sqrt{k}}\cos\left(\int\limits_0^x kdx - \frac{\pi}{4}\right)$$

в согласии с (3.9).

Условие квантования

Квазиклассическое решение уравнения Шредингера в классически доступной области ($x_1 < x < x_2$; рис. 26) можно записать двумя способами: один раз - сшивая осциллирующее решение с затухающим в точке x_1, а другой раз - в точке x_2. Требование совпадения этих двух функций и даст нам условие квантования.

Первое из решений имеет вид

$$\varphi_1 = \frac{a_1}{\sqrt{k}}\cos\left(\int\limits_{x_1}^x kdx - C_1\pi\right),$$

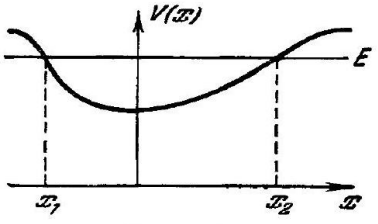


Рис. 26.

где $C_1\pi -$, которая возникает при сшивке с затухающей экспоиентой для $x < x_1$. В тех случаях, когда потенциал в окрестности точки x_1 имеет линейный ход, получается, как мы видели, $C_1 = 1/4$.

Второе из решений имеет вид

$$\varphi_2 = \frac{a_2}{V/k} \cos\left(\int_x^{x_2} k dx - C_2\pi\right).$$

Условие совпадения решений даст

$$\int_{x_1}^{x_2} k dx = (n + C_1 + C_2)\,\pi$$

(при этом $a_1 = a_2(-1)^n$).

Нетрудно видеть, что $\cos\left(\int_{x_1}^{x} k dx - C_1\pi\right)$ проходит через нуль n раз, т. е. n-число узлов волновой функции в интервале $[x_1, x_2]$.

Проверим правило квантования (3.14) (так называемое правило квантования Бора) на примере одномерной прямоугольной ямы с бесконечно высокими стенками. Так как волновая функция должна обращаться в нуль как на левой, так и на правой границах, то $C_1 = C_2 = 1/2$. Получаем

$$\int_{x_1}^{x_2} k_n dx = k_n L = (n-1)\pi, \quad E_n = \frac{1}{2}k_n^2 = \frac{\pi^2}{2L^2}(n+1)^2,$$

где L - длина ямы. Наинизшему состоянию соответствует число узлов $n = 0$.

В наиболее частом слуцае, когда потенциал имеет линейный ход как вблизн x_1, так и вблизи x_2, получаем правило квантования

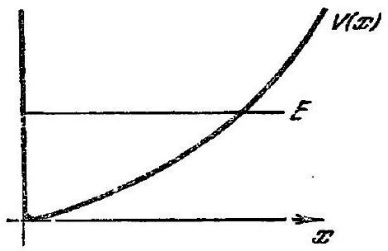


Рис. 27.

$$\int_{x_1}^{x_2} k dx = \left(n + \frac{1}{2}\right)\pi.$$

Мы увидим ниже (стр. 137), что применение квазиклассического приближения для радиальной кулоновской функции при $l = 0$ дает $C_1 = 3/4, \quad C_2 = 1/4$ а при $l \neq 0 \quad C_1 = C_2 = 1/4$.

3 ад ч а. Показать, что для потенциала, нзображенного на рис. 27, условие квантования имеет вид

$$\int_{x_1}^{x_2} k dx = \left(n + \frac{3}{4}\right)\pi.$$

Точность кваєинлассического приблинения

Едйнственное приближение, которое мы делали при выводе наших формул, состояло в отбрасывании слагаемого

$$\frac{A''}{k^2 A} \sim \frac{A/l^2}{k^2 A} \sim \frac{1}{(kl)^2}.$$

Дlя оценки kl заметим, что

$$\int k dr \sim kl \sim n\pi,$$

где n - число узлов. Следовательно, квазиклассическое прин ближение справедливо. с точностью до $1/\pi^2 n^2$ (а не $1/n$). Ɣimенно поэтому в правиле квантования Бора законно сохранять добавку $1/2$ кислу узлов , которая иредставляет собон(??) поправку $\sim 1/n$.

Нормяровка квазиклассических функций

Сунественший вклад в пориировопный интеграл внесет лишь область $x_1 < x < x_2$ (см. рис. 26), так как вне ее волновая функция экспоненциально затухает. При $x_1 < x < x_2$ волновая функция

$$\varphi_n = \frac{a}{\sqrt{\dot{\alpha}}} \cos\left(\int_{x_1}^{x} k dx - \frac{\pi}{4}\right)$$

следовательно,

$$\int |\varphi_n|^2 dx = 1 \approx \int_{x_1}^{x_2} \frac{a^2}{h} \cos^2 \Phi dx$$

где

$$D = \int_{x_1}^{x} k dx - \frac{\pi}{4}$$

Гри $E = E_n$ волновая функция φ_n имеет n узлов в области $[x_1, x_2]$, так как $\int_{x_1}^{x_2} kax$ изменяется от нуля до $(n + 1/2)\pi$ и cos Φ будет n раз обраныться в нуль. Если n велико, то фаза D - большое число.

Далее, $\cos^2 \mathrm{D} = \frac{1}{2} + \frac{1}{2}\cos 2\mathrm{D}$. Второе слагаемое много раз изменяет знак и поэтому внесет малый вклады. Следовательно,

$$1 \approx \frac{a^2}{2} \int_{x_1}^{x_2} \frac{dx}{k} = \frac{a^2}{2}\frac{T}{2},$$

где T-период классиического движения. Мтак,

$$\alpha^2 = -\frac{4}{T} = \frac{2}{\pi}\omega,$$

где ω - частота колебаний в соответствующей классической задаче. Таким образом,

$$\varphi_n = \sqrt{\frac{2\omega}{\pi k}} \cos\left(\int_{x_1}^{x} k dx - \frac{\pi}{4}\right).$$

3 адача. Оценить вклад в нормировочный множитель от классически недоступной области. О т в т.

$$1/(\pi n)^{1/3}$$

Принцип соответствия

Из правила квантования (3.9), дифференцированием по n получаем

$$\pi = \frac{d\varepsilon_n}{dn} \int_{x_1}^{x_3} \frac{dx}{k} = \frac{d\varepsilon_n}{dn} \frac{\pi}{\omega},$$

откуда

$$\frac{d\varepsilon_n}{dn} = \omega$$

Это соотношение называется принципом соответствия: при больших квантовых числах разность соседних уровней энергии равна классической частоте движения.

Средняя кинетическая энергия

Выразим среднюю кинетическую энергию частицы при квазиклассическом движении через ее иолную энергию:

$$\bar{T} = \frac{1}{2}\int \varphi_n^* \hat{p}^2 \varphi_n \, dx = -\frac{1}{2}\int \varphi_n^* \frac{d^2}{dx^2} \varphi_n \, dx \approx \frac{1}{2}\int \varphi_n^* k^2 \varphi_n \, dx.$$

3 десь величина k - число, а не оператор. Дифференцированне $1/\sqrt{k}$ в $\varphi_n = \frac{a}{\sqrt{k}} \cos\left(\int_{x_1}^{x} k dx - \frac{\pi}{4}\right)$ вносит малый вклад в $\bar{T}$. Используя (3.16), получим

$$\bar{T} = \frac{a^2}{2} \int_{x_1}^{x_2} k^2 \frac{1}{k} \cos^2 \Phi dx = \frac{a^2}{4} \int_{x_1}^{x_2} k dx =$$
$$= \frac{a^2}{4}\left(n + \frac{1}{2}\right)\pi = \frac{1}{2}\left(n + \frac{1}{2}\right)\frac{d\varepsilon_n}{dn}.$$

В случае кулоновского потенциала при $l = 0$ условие квантования не содержит $1/2$ и

$$\bar{T} = \frac{1}{2} n \frac{d\varepsilon_n}{dn}.$$

Если принять во внимание теорему вириала

$$\bar{T} = \frac{1}{2}\overline{x\frac{dV}{dx}},$$

то из (3.17) и (3.19) можно найти собственные значения энергии в квазиклассическом случае. Например, для осциллятора $V \sim x^2$ и $\overline{x\frac{dV}{dx}} = 2\bar{T}$, т. е. $\bar{T} = \bar{V}$. Следовательно,

$$\left(n + \frac{1}{2}\right)\frac{d\varepsilon_n}{dn} = \varepsilon_n.$$

Решая это уравнение, получим $\varepsilon_n = C(n+1/2)$. Из принципа соответствия следует, что $C = \omega$ - частоте классического движения, следовательно, $\varepsilon_n = (n + {}^1/2)\,\omega$. Д алее, для кулоновского потенциала при $l = 0$ из (3.18) и (3.19): $\bar{T} = -1/2\bar{V} = \frac{1}{2}n\frac{d\varepsilon_n}{dn}, \varepsilon_n = \bar{T} - 2\bar{T} = -\bar{T} = -\frac{1}{2}n\frac{d\varepsilon_n}{dn}$.Ре - шение этого уравнения есть $\varepsilon_n = C/n^2$. Мы видели (стр. 36), что из принципа соответствия следует $C = -1/2$.

Связь квазиклассических матричных элементов с компонентами Фурье классического движения

Свяжем матричный элемент $\int \varphi_n^* U(x)\varphi_n dx$ одномерной задачи с компонентой Фурье от классической величины $U[x(t)]$ (например, дипольный матричный элемент

$$\int \varphi_n^* x \varphi_n dx$$

можно связать с компонентой Фурье классической координнаты движения $x(t)$).

Пусть n' не очень снльно отличаются друг от друга, именно,

$$\frac{|n'-n|}{n} \ll 1, \quad n \geqslant 1, \quad n' \geqslant 1.$$

тогда матричный элемент
$U_{nn'} = \int \varphi_n^* U \varphi_{n'} dx = a_n a_{n'} \int \frac{U}{\sqrt{kk'}} \cos\Phi_n \cos\Phi_{n'} dx =$

$$= a_n^2 \int U\left[\cos\left(\Phi_n - \Phi_{n'}\right) + \cos\left(\Phi_n + \Phi_{n'}\right)\right]\frac{dx}{2k}.$$

Так как Φ_n и Φ_n в велики, то второе слагаемое в подынтегральном выражелии можно отбросить из-за сильной осцилляции $\cos\left(\Phi_n + \Phi_{n'}\right)$. Следовательно,

$$U_{nn'} = \frac{a_n^2}{2}\int\limits_{x_1}^{x_2} U(x)\cos\left(\phi_n - \mathrm{i}_{n'}\right)\frac{dx}{v}.$$

Так как
$\Phi_n - \lesseqgtr_{n'} = \int\limits_{x_{ib}}^{x} t_n dx - \int\limits_{x'_{ib}}^{x} k_{n'} dx \approx \int\limits_{x_{ii}}^{x} \frac{d_{ni}}{i_n}\left(\varepsilon_n - \varepsilon_{n2'}\right) =$

$$= \frac{d\varepsilon_n}{dn}\left(n - n'\right)\int\limits_{x_i}^{x}\frac{dx}{v} = \frac{d\varepsilon_n}{dn}\left(n-n'\right)t,$$

ТО

$$U_{nn} = \frac{2}{T}\int\limits_0^{T/2} U[xt]\Bigg]\cos\frac{2\pi\left(n-n'\right)t}{T}dt.$$

Итак, матричный элемент величины $U(x)$ в квазиклассическом приближении равен фууре-компоненте величины $U[x(t)]$.

Критерйй применимости теории возмуаений расqета не слинком налых величин

При возмущении -го состояния дискретного сиектра критерий применимости теории возмущений имеет вид $H' < E_{nm}$, гпе H' - матричный элсмент возмущения, а $E_{nm} = E_n - E_m$. Здесь E_n и E_m означают ближайшие уровни, для которьх матричный элемент H'_{nm} не мал. Так как

$$E_{nm} \sim \frac{dE_n}{dn} \sim \frac{E_n}{n},$$

где n-число узлов волновой функции, то это условие сводится к

$$\frac{H'}{E_n} n \ll 1.$$

В квазиклассическом случае $n \gg 1$, и это условие.может не выполняться. Покажем, что для вычисления не слишком малых величин его можно заменить более мягким условием:

$$\frac{H'}{E_n} \leqslant 1.$$

Для доказательства этого утверждения рассмотрим матричный элемент $U_{nm} = (\varphi_n|U|\varphi_{mn})$. ГIусть $U(x)$ - плавная функция. Тогда $U_{nm} \neq 0$, лиць когда n и m мало отличаюгся друг. от друга (иначе у подынтегральной функции будет много узлов). Воспользовазцись квазиклассическими волновыми функіцияи, полугаем

$U_{nm} \approx \frac{a_n a_{in}}{2} \int U(x) \frac{dx}{\sqrt{k_n k_m}} \{\cos(\Phi_n - \Phi_m) + \cos(\Phi_n + \Phi_m)\}$.

Второе слагаемое в подынтегральном выражении для U_{nm} осциллирует $n + m$ раз, поэтому его вкладом можно пренебречь. Следовательно,

$$U_{nm} \approx \frac{a_n a_m}{2} \int U(x) \frac{\cos(\Phi_n - \Phi_m)}{\sqrt{k_n k_m}} dx.$$

Пусть теперь к потенциалу $V(x)$ добавляется малая величина $H'(x)$. Так как $k_n = \sqrt{2[E_n - V(x)]}$, то

$$\Delta k_n = \sqrt{2[E_n - V(x) - H'(x)]} - \sqrt{2[E_n - V(x)]} \sim \frac{H'}{k_n},$$

следовательно, $\Delta k_n/k_n \sim H'/k_n^2 \sim H'/E_n$, если V не близко к E_n (иначе квазнклассика неприменима). Следовательно, условиее $\Delta k_n/k_n \ll 1$ эквивалентно $H'/E_n \ll 1$, Т. е. изменением k можно пренебречь при вынолнении условия (3.21). При вычислении фазы $\Phi_n = \int\limits_{x_1}^{x} k_{nz} dx - \frac{\pi}{4}$ этого нельзя делать, так как $\delta\Phi_n \approx \int\limits_{x_1}^{x} \delta k_n dx \approx \int \frac{H'}{E_n} k_n dx \sim \frac{H'}{E_n} n$, где n-число узлов. Поэтому условие $\delta\Phi_n \ll 1$ означает $\frac{H'}{E_n} n \ll 1$; отсюда и возник критерий теории возмущений.

Однако мы видим, что для вычисления величин, содержащих $\Phi_n - \Phi_m$, причем $|n-m| \sim 1$, изменение разности Фаз имеет порядок

$$\delta\left(\bar{\Phi}_n - \Phi_m\right) \sim \frac{H'}{E_n}(n-m) \sim \frac{H'}{E_n}.$$

Следовательно, изменение больших матричных элементов U_{nm} гпри возмуцении потенциала на величину $H'(x)$ определяется условием $H'/E_n \ll 1$, что и нужно было показать.

Если $|n - m|$ не мало, то изучаемый матричный элемент мал из-за осцилляций $\cos(\Phi_n - \Phi_m)$.

Выясним, как изменяется квазиклассическая волновая функция $\Psi = Ae^{is}$ при добавлении малой величины $H'(x)$ к потенциалу $V(x)$. Мзменение A определяется величиной H'/E, поскольку $A \sim 1/\sqrt{k}$, а $\Delta k/k \sim H'/E$, как уже было найдено. Но $S = \int k dl$, поэтому $\delta S \sim n\frac{H'}{E}$, так что δS может быть и больне 1, хотя $H'/E \ll 1$. Мзменение Ψ при добавлении H' равно:

$$\delta\Psi \approx \Psi e^{i\delta S} \approx \Psi \exp\left(-\int \frac{H' dx}{k}\right)$$

Возмущение, вызываемое деформацией ядра, не удовлетворяет критерию (3.20), но критерий (3.21) выполняется. Поэтому для вычисления не очень малых величин можно пользоваться теорией возмущении (стр. 74).

Надбарьерное отражение

Решим задачу об отражении частицы при движении с энергией, больцей высоты барьера, так что везде выполняется критерий квазиклассического приближеция. Легко увидеть, что ни в каком приближении по параметру квази- классичности $1/(kl)^2$ не возникает отраженной волны. Действительно, квазиклассическое приближение, соответствующее идуцей направо волне, имеет вид

$$A \exp\left[i \int_{x_1}^{x} \sqrt{k^2 + A''/A} dx \right].$$

Разлагая это решение по степеням A''/A, получим всюду только волны, идушие вправо.

Причина этого результата в том, что коэффициент отражения экспоненциально падает с увеличением $(kl)^2$, между тем как квазиклассическое решение есть асимптотический ряд и экспоненциально малые добавки в нем полностью теряются.

Lелесообразно искать решение уравнения Шредингера

$$\Psi' + k^2(x)\Psi = 0$$

В Виде

$$\Psi = \sqrt{\frac{k_0}{k}} \exp\left(i \int_{-\infty}^{x} k dx \right) + \varphi$$

где φ - малая добавка, содержашая отраженнуго волну.

Тогда получаем

$$\varphi'' + k^2 \varphi = f(x)$$

rale

$$f(x) = -A'' \exp\left[i \int_{-\infty}^{x} k dx \right]$$

Выразим решение этого неоднородного уравнения через два решения соответствующего однородного уравнения Ψ_1 и Ψ_2(Ψ_1 и Ψ_2 $\rightarrow$ волны, идущие соответственно вправо и влево):

где

$$\varphi = \frac{1}{\Delta} \left\{ \Psi_1 \int^{x} \Psi_2 f dx - \Psi_2 \int_{1}^{x} \Psi_1 f dx \right\}$$

$$\Delta = \Psi_1' \Psi_2 - \Psi_1 \Psi_2' = \text{ const}$$

- онределитель Вронского.

Цтак, решение уравнения LЦредингера (3.23) имеет вид

$$\Psi(x) = \sqrt{\frac{\widehat{k_0}}{k}} \exp\left[i \int\limits_{-\infty}^{x} k dx\right] +$$

$$+ \frac{1}{\Delta}\left\{\Psi_1 \int\limits_{-\infty}^{x} \Psi_2 f dx - \Psi_2 \int\limits_{-\infty}^{x} \Psi_1 f dx\right\}.$$

Пределы интегрирования определяются из следующих соображений: при $x \longrightarrow \infty$ должна оставаться только волна, идущая вправо; это обеспечивается функцией Ψ_1. I1ри $x \to -\infty$ функция $\varphi(-\infty)$ должна содержать только отраженную волну. Действительно, при указанном выборе нижнего предела

$$\Psi(x) \underset{x\to-\infty}{=} e^{ik_0 x + i\alpha} + \frac{1}{\Delta} e^{-ik_0 x} \int\limits_{-\infty}^{\infty} \Psi_1 f dx.$$

Так как $\Delta = \text{const}$, можно вычислить Δ при $x \longrightarrow \infty$. Функция $\Psi_1 \longrightarrow e^{ik_0 x}$, а функция Ψ_2 в силу малого коэффициента отражения приближенно стремится к $e^{-ik_0 x + i\alpha}$. Отсюда $|\Delta| = 2k_0$.

Таким образом, коэффициент отраяения

$$R = \left|\frac{1}{\Delta} \int\limits_{-\infty}^{\infty} \Psi_1 f dx\right|^2 = \left|\frac{1}{2k_0} \int\limits_{-\infty}^{\infty} \Psi_1 f dx\right|^2.$$

Заметим, что в (3.24) не используется квазиклассическое приближение.

Если $V \ll E$, то из (3.24) получается обычная формула теории возмущений. Действительно, величина $A' = -\frac{\sqrt{k_0}}{2\sqrt{k^3}} k'$. Так как $k = \sqrt{2(E-V)}$, то $k' = -V'/k$, следовательно, $f = -A'' e^{iS} \approx \frac{V''}{2k_0^2} e^{ik_0 x + i\alpha}$ и

$$R = \left|\frac{1}{4k_0^3} \int\limits_{-\infty}^{\infty} V'' e^{2ik_v x} dx\right|^2.$$

Iинтегрируя дважділ по частим, попучим выражение для коэффициента отражения, совиадающее стем, что получается по теории возмущений

$$R = \left|\frac{1}{k_0} \int\limits_{-\infty}^{\infty} V e^{2ik_0 x} dx\right|^2.$$

Величина R определяется поведением $\Psi_1 f$ в окрестности ближайшєй к вещественной оси особой точки.

6.9.5 Time-Dependent Asymptotics by Takhtajan

Здесь мы опишем соотношение между классической и квантовой механикой, рассмотрев поведение волновой функции $\psi(\boldsymbol{q}, t)$ - решения зависящего от времени уравнения Шрёдингера [10]

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta\psi + \dot{V}(\boldsymbol{q})\psi$$

при $\hbar \to 0$. Подстановка

$$\psi(\boldsymbol{q}, t) = e^{-\frac{i}{\hbar} S(\boldsymbol{q}, t; \hbar)}$$

сводит (6.1) к следующему нелинейному уравнению в частных производных:

$$\frac{\partial S}{\partial t} + \frac{1}{2m} \left(\frac{\partial S}{\partial \boldsymbol{q}} \right)^2 + V(\boldsymbol{q}) = \frac{i\hbar}{2m} \Delta S$$

Замечательно, что (6.3) отличается от уравнения Гамильтона- Якоби (2.4) для функции Гамильтона $H_c(\boldsymbol{p}, \boldsymbol{q}) = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{q})$, рассмотренной в разделе 1.2.3 главы 1, только слагаемым в правой части, пропорциональным $\hbar$. Таким образом, при $\hbar \to 0$ уравнения движения квантовой механики переходят в классические уравнения движения.

Для стационарного состояния $\psi(\boldsymbol{q}, t) = \psi(\boldsymbol{q}) e^{-\frac{i}{\hbar} Et}$ подстановка (6.2) превращается в

$$\psi(\boldsymbol{q}, t) = e^{-\frac{i}{\hbar} (\sigma(\boldsymbol{q}; \hbar) - Et)}$$

Соответствующее нелинейное уравнение в частных производных:

$$\frac{1}{2m} \left(\frac{\partial \sigma}{\partial \boldsymbol{q}} \right)^2 + V(\boldsymbol{q}) = E + \frac{i\hbar}{2m} \Delta \sigma$$

отличается от соответствующего уравнения Гамильтона-Якоби для укороченного действия, рассмотренного в разделе 1.2.5 главы 1, пропорциональным $\hbar$ слагаемым в правой части.

[10] Здесь будет удобно обозначать декартовы координаты на $\mathbb{R}^n$ как $\boldsymbol{q} = (q_1, ..., q_n)$. В этом разделе мы рассмотрим квазиклассическую асимптотику: асимптотики уравнений в частных производных (6.3) и (6.5) при $\hbar \to 0$. Они описывают точное соотношение между квантовой и классической механикой и представляют количественную форму принципа соответствия, обсуждавшегося в разделе 2.2 главы 2. В частности, используя квазиклассическую асимптотику стационарного уравнения Шрёдингера, мы выведем правила квантования Бора- Вильсона - Зоммерфельда, которые были постулированы в разделе 2.2.5 главы 2.

Theory

Здесь мы рассмотрим задачу нахождения коротковолновой асимптотики - асимптотики при $\hbar \to 0$ решения $\psi_\hbar(q, t)$ задачи Коши для одномерного уравнения Шрёдингера (6.1),

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial q^2} + V(q)\psi$$

с начальным условием

$$\psi_\hbar(q, t)|_{t=0} = \varphi(q) e^{\frac{i}{\hbar} s(q)}$$

Предполагается, что вещественнозначные функции $\varphi(q)$ и $s(q)$ - гладкие, $s(q), \varphi(q) \in C^\infty(\mathbb{R})$ и что у «амплитуды» $\varphi(q)$ компактный носитель. Подстановка (6.2) - это $\psi_\hbar(q, t) = e^{\frac{i}{\hbar} S(q, t, \hbar)}$, и дифференциальное уравнение (6.3) принимает вид

$$\frac{\partial S}{\partial t} + \frac{1}{2m} \left(\frac{\partial S}{\partial q} \right)^2 + V(q) = \frac{i\hbar}{2m} \frac{\partial^2 S}{\partial q^2}$$

Чтобы определить асимптотическое поведение $S(q, t, \hbar)$ при $\hbar \to 0$, предположим, что при $\hbar \to 0$

$$S(q,t,\hbar)=\sum_{n=0}^{\infty}(-i\hbar)^n S_n(q,t),$$

и подставим это разложение в (6.6). Сравнивая члены с одинаковыми степенями $\hbar$, получим, что $S_0(q,t)$ удовлетворяет задаче с начальными условиями

$$\frac{\partial S_0}{\partial t}+\frac{1}{2m}\left(\frac{\partial S_0}{\partial q}\right)^2+V(q)=0$$

И

$$S_0(q,t)|_{t=0}=s(q)$$

где $S_1(q,t)$ удовлетворяет дифференциальному уравнению

$$\frac{\partial S_1}{\partial t}+\frac{1}{m}\frac{\partial S_0}{\partial q}\frac{\partial S_1}{\partial q}=-\frac{1}{2m}\frac{\partial^2 S_0}{\partial q^2}$$

так называемому транспортному уравнению, и

$$S_1(q,t)|_{t=0}=\log\varphi(q)$$

Функции $S_n(q,t)$ при $n>1$ удовлетворяют неоднородным дифференциальным уравнениям, подобным (6.9).

Задача с начальными условиями (6.7) - (6.8) - это задача Коши для уравнения Гамильтона - Якоби с функцией Гамильтона

$$H_c(p,q)=\frac{p^2}{2m}+V(q)$$

рассмотренной в разделе 1.2.3 главы 1. Согласно предложению 2.1 в разделе 1.2.3 главы 1, решение уравнений (6.7) – (6.8) получается методом характеристик:

$$S_0(q,t)=s\left(q_0\right)+\int_0^t L\left(\gamma'(\tau)\right)d\tau$$

Здесь $L(q,\dot q)\doteq\frac{1}{2}m\dot q^2-V(q)$ - функция Лагранжа, а $\gamma(\tau)$ - характеристика, классическая траектория, начинающаяся в точке q_0 в момент времени $\tau=0$ с импульсом $p_0=\frac{\partial s}{\partial q}\left(q_0\right)$ и заканчивающаяся в точке q в момент $\tau=t$, где q_0 однозначно определяется из q. (Мы предполагаем, что гамильтонов фазовый поток g_t удовлетворяет предположениям, сделанным в разделе 1.2.3 главы 1.) Из теоремы 2.7 в разделе 1.2.3 главы 1 следует, что на характеристике

$$\frac{\partial S_0}{\partial q}(q,t)=m\frac{d\gamma}{dt}(t)$$

так что

$$\left(\frac{\partial}{\partial t}+\frac{1}{m}\frac{\partial S_0}{\partial q}\frac{\partial}{\partial q}\right)S_1(\gamma(t),t)=\frac{d}{dt}S_1(\gamma(t),t)$$

Тепіерь мы можем решить задачу Коши (6.9) – (6.10) для транспортного уравнения явным образом. Рассмотрим поток $\pi_t:\mathbb{R}\to\mathbb{R}$, определенный в разделе 1.2.3 главы 1, и обозначим [11] как $\gamma(Q,q;\tau)$ характеристику, соединяющую точки q в момент $\tau=0$ и $Q=\pi^t(q)$ в момент $\tau=t$ (при наших предположениях, что поток π_t - диффеоморфизм и отображение $q\mapsto Q$ взаимно однозначно). Дифференцируя уравнение

$$\frac{\partial S_0}{\partial Q}(Q,t) = m\frac{\partial \gamma}{\partial t}(Q,q;t)$$

по q, получаем

$$\frac{\partial^2 S_0}{\partial Q^2}(Q,t)\frac{\partial Q}{\partial q} = m\frac{\partial^2 \gamma}{\partial q \partial t}(Q,q;t) = m\frac{d}{dt}\left(\frac{\partial Q}{\partial q}\right)$$

так что (6.9) можно переписать как

$$\frac{d}{dt}S_1(Q,t) = -\frac{1}{2}\frac{d}{dt}\log\frac{\partial Q}{\partial q}$$

и, используя (6.10), получаем

$$S_1(Q,t) = \varphi(q)\left|\frac{\partial Q}{\partial q}(q)\right|^{-\frac{1}{2}}$$

Поэтому

$$\psi_\hbar(Q,t) = \varphi(q)\left|\frac{\partial Q}{\partial q}(q)\right|^{-\frac{1}{2}} e^{\frac{i}{\hbar}(S(Q,q;t)+s(q))}(1+O(\hbar)),$$

где $S(Q,q;t)$ - классическое действие на характеристике, начинающейся в точке q в момент $\tau = 0$ и кончающейся в точке Q в момент $\tau = t$.

Строгое доказательство того, что (6.13) - асимптотическое разложение при $\hbar \to 0$, использует предположения, сделанные в разделе 1.2.3 главы 1, и оставляется заинтересованному читателю. Здесь мы только заметим, что асимптотика (6.13) согласуется с сохранением вероятности: для любого борелевского подмножества $E \subset \mathbb{R}$

$$\int\limits_{E_t} |\psi_\hbar(Q,t)|^2\, dQ = \int\limits_{E} |\varphi(q)|^2 dq + O(\hbar)$$

при $\hbar \to 0$, где $E_t = \pi_t(E)$.

[11] Не путать с оператором квантовой координаты Q. ЗАМЕчАНИЕ. Когда предположения раздела 1.2.3 главы 1 не выполняются, ситуация становится более сложной. А именно: в этом случае может быть несколько характеристик $\gamma_j(\tau)$, которые заканчиваются в точке Q при $\tau = t$, имея q_j своими соответствующими начальными точками. Тогда

$$\psi_\hbar(Q,t) = \sum_j \varphi(q_j)\left|\frac{\partial Q}{\partial q}(q_j)\right|^{-\frac{1}{2}} e^{\frac{i}{\hbar}(S(Q,q_j;t)+s(q_j))-\frac{\pi i}{2}\mu_j}(1+O(\hbar))$$

где $\mu_j \in \mathbb{Z}$ - индекс Морса характеристики γ_j. Он определяется как число фокальных точек на фазовой кривой $(q(\tau),p(\tau))$ с начальными данными q_j и $p_j = \frac{\partial s}{\partial q}(q_j)$ по отношению к конфигурационному пространству $\mathbb{R}$. Это частный случай более общего индекса Маслова.

Случай n степеней свободы рассматривается похоже. При предположениях раздела 1.2.3 главы 1 решение $\psi_\hbar(\boldsymbol{q},t)$ уравнения Шрёдингера (6.1) с начальным условием

$$\psi_\hbar(\boldsymbol{q},t)|_{t=0} = \varphi(\boldsymbol{q})e^{\frac{i}{\hbar}s(\boldsymbol{q})}$$

где вещественнозначные функции $s(\boldsymbol{q})$ и $\varphi(\boldsymbol{q})$ - гладкие, а $\varphi(\boldsymbol{q})$ - еще и с компактным носителем, имеет следующую асимптотику при $\hbar \to 0$:

$$\psi_\hbar(\boldsymbol{Q},t)=\varphi(\boldsymbol{q})\left|\det\left(\frac{\partial \boldsymbol{Q}}{\partial \boldsymbol{q}}(\boldsymbol{q})\right)\right|^{-\frac{1}{2}} e^{\frac{i}{\hbar}(S(\boldsymbol{Q},\boldsymbol{q};t)+s(\boldsymbol{q}))}(1+O(\hbar))$$

6.9.6 Time-Independent Asymptotics

Здесь мы рассмотрим квазиклассическую асимптотику для одномерного уравнения Шрёдингера

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi$$

Этот асимптотический метод известен также как метод BKD (в честь Дж. Венцеля, Х. Крамерса и Л. Бриллюэна). Подстановка (6.4) - это $\psi_\hbar(x)=e^{\frac{i}{\hbar}\sigma(x;\hbar)}$, и уравнение (6.5) принимает вид

$$\frac{1}{2m}\left(\frac{d\sigma}{dx}\right)^2+V(x)=E+\frac{i\hbar}{2m}\frac{d^2\sigma}{dx^2}$$

Как и в предыдущем разделе, воспользуемся разложением

$$\sigma(x,\hbar)=\sum_{n=0}^{\infty}(-i\hbar)^n\sigma_n(x)$$

и для первых двух членов получим

$$\frac{1}{2m}\sigma_0'^2=E-V(x)\quad\text{ и }\quad\sigma_0'\sigma_1'=-\frac{1}{2}\sigma_0''$$

Пусть $p(x)=\sqrt{2m(E-V(x))}$ - классический импульс частицы, движущейся в потенциале $V(x)$ с энергией E. Решение первого уравнения в (6.16) дается формулой

$$\sigma_0=\pm\int p(x)dx$$

а из второго уравнения в (6.16) мы получаем

$$\sigma_1=-\frac{1}{2}\log p$$

Волновая функция в приближении ВКБ имеет вид

$$\psi_\hbar(x)=\frac{1}{\sqrt{|p(x)|}}\left(C_1e^{\frac{i}{\hbar}\int p(x)dx}+C_2e^{-\frac{i}{\hbar}\int p(x)dx}\right)(1+O(\hbar))$$

где $p(x)$ вещественно в классической области $V(x)<E$ и чисто мнимо в классически недоступной области $V(x)>E$ (см. раздел 1.1.5 главы 1).

Заметим, что асимптотика (6.17) верна, только если $\hbar|\sigma''|\ll(\sigma')^2$, что в первом приближении дает

$$\left|\frac{d}{dx}\left(\frac{\hbar}{p(x)}\right)\right|\ll 1$$

Введя классическую силу $F=-\frac{dV}{dx}$, это условие можно переписать как

$$\frac{m\hbar F}{p^3}\ll 1$$

Таким образом, приближение ВКБ не работает, когда классический импульс $p(x)$ мал. В частности, оно неприменимо вблизи точек поворота, где $E = V(x)$, и поэтому $p(x) = 0$. Пусть $x = a$ - точка поворота. Если $F_0 = F(a) \neq 0$, то, используя приближение $E - V(x) \simeq F_0(x - a)$ вблизи $x = a$, можно заменить (6.15) уравнением

$$\frac{\hbar^2}{2m}\psi'' = F_0(x - a)\psi.$$

Это дифференциальное уравнение в явном виде решается методом Лапласа. Его ограниченное решение - это

$$\psi(x) = \Phi(\xi), \quad \xi = \left(\frac{2mF_0}{\hbar^2}\right)^{\frac{1}{3}}(a - x)$$

где $\Phi(\xi)$ - функция Эйри - Фока, определенная несобственным интегралом

$$\Phi(\xi) = \frac{1}{\sqrt{\pi}}\int\limits_0^\infty \cos\left(\frac{1}{3}t^3 + \xi t\right)dt$$

Асимптотика функции Эйри-Фока при больших ξ, полученная методом перевала, следующая:

$$\Phi(\xi) = \frac{1}{2\sqrt[4]{\xi}}e^{-\frac{2}{3}\xi^{\frac{3}{2}}}\left(1 + O\left(\xi^{-\frac{3}{2}}\right)\right) \quad \text{при} \quad \xi \to \infty$$
$$\Phi(\xi) = \frac{1}{\sqrt[4]{|\xi|}}\sin\left(\frac{2}{3}|\xi|^{\frac{3}{2}} + \frac{\pi}{4}\right)\left(1 + O\left(|\xi|^{-\frac{3}{2}}\right)\right) \quad \text{при} \quad \xi \to -\infty$$

Используя асимптотику (6.19) - (6.20), можно получить формулы, связывающие приближения ВКБ для классической и недоступной областей. Строгое обоснование этого подхода технически достаточно трудоемко, и мы не будем приводить его здесь. Вместо этого мы обсудим простейший случай, когда имеется только одна точка поворота $x = a$ с $F_0 > 0$, так что $x < a$ - классически недоступная область. Из (6.17) получаем, что волновая функция ВКБ в недоступной области $x < a$ экспоненциально затухает:

$$\psi_{\text{wKB}}(x) = \frac{A}{\sqrt{|p(x)|}}e^{\frac{1}{\hbar}\int\limits_a^x |p(s)|ds}$$

тогда как в классической области $x < a$ - осциллирует:

$$\psi_{\text{wKB}}(x) = \frac{1}{\sqrt{p(x)}}\left(C_1 e^{\frac{i}{\hbar}\int\limits_a^x p(s)ds} + C_2 e^{-\frac{i}{\hbar}\int\limits_a^x p(s)ds}\right) = \frac{B}{\sqrt{p(x)}}\sin\left(\frac{1}{\hbar}\int\limits_a^x p(s)ds + \alpha\right)$$

Как следует из (6.18), приближение ВКБ вблизи точки поворота $x = a$ остается уместным при $|x - a| \gg \frac{1}{2}\left(\frac{\hbar^2}{mF_0}\right)^{\frac{1}{3}}$, что эквивалентно условию $|\xi| \gg 1$. С другой стороны, когда $|x - a| \ll 1$, волновая функция имеет асимптотику

$$\psi_\hbar(x) = C\Phi(\xi)(1 + O(\hbar))$$

Чтобы определить неизвестную фазу α и найти соотношения между коэффициентами A, B и C, рассмотрим область $\frac{1}{2}\left(\frac{\hbar^2}{mF_0}\right)^{\frac{1}{3}} \ll |x - a| \ll 1$ и сравним приближение ВКБ для

волновой функции с асимптотикой функции Эйри-Фока при больших ξ. А именно: при $x < a$ имеем $\xi \gg 1$ и

$$\frac{2}{3}\xi^{\frac{3}{2}} = \frac{2}{3\hbar}\sqrt{2mF_0}(a-x)^{\frac{3}{2}} \simeq \frac{1}{\hbar}\int\limits_x^a |p(s)|ds, \quad \sqrt[4]{\xi} = \frac{\sqrt{|p(x)|}}{\sqrt[6]{2m\hbar F_0}}$$

Сравнивая (6.19) с волновой функцией ВКБ при $x < a$, получаем, что $2A = \sqrt[6]{2m\hbar F_0}C$. При $x > a$ имеем $\xi \ll -1$ и

$$\frac{2}{3}|\xi|^{\frac{3}{2}} = \frac{2}{3\hbar}\sqrt{2mF_0}(x-a)^{\frac{3}{2}} \simeq \frac{1}{\hbar}\int\limits_a^x p(s)ds, \quad \sqrt[4]{|\xi|} = \frac{\sqrt{p(x)}}{\sqrt[6]{2m\hbar F_0}}$$

Сравнивая (6.20) с волновой функцией ВКБ при $x < a$, получаем, что $\alpha = \frac{\pi}{4}$ и $B = \sqrt[6]{2m\hbar F_0}C$, так что $B = 2A$. Таким образом, в этом примере волновая функция ВКБ - это

$$\psi_{\text{wKB}}(x) = \begin{cases} \frac{A}{\sqrt{|p(x)|}} e^{\frac{1}{\hbar}\int\limits_a^x |p(s)|ds}, & \text{когда } x < a, \\ \frac{2A}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int\limits_a^x p(s)ds + \frac{\pi}{4}\right), & \text{когда } x > a. \end{cases}$$

Случай, когда имеется только одна точка поворота $x = b$ с $F_0 < 0$, так что $x > b$ - классически недоступная область, сводится к предыдущему примеру с помощью изменения ориентации $x \mapsto -x$. Как результат, получаем

$$\psi_{\text{wB}}(x) = \begin{cases} \frac{2B}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int\limits_x^b p(s)ds + \frac{\pi}{4}\right), & \text{когда } x < b, \\ \frac{B}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int\limits_b^x |p(s)|ds}, & \text{когда } x > b. \end{cases}$$

ЗАДАЧА 6.1 (ПРОХОЖДЕНИЕ ЧЕРЕЗ ПОТЕНЦИАЛЬНЫЙ БАРЬЕР). Рассмотрим потенциальный барьер для заданной энергии E - потенциал $V(x)$, такой, что $\{x \in \mathbb{R} : V(x) > E\} = (a, b)$. Покажите, что

$$T_{\text{WKB}} = e^{-\frac{2}{\hbar}\int\limits_a^b |p(x)|dx}$$

Проверьте непосредственно, что коэффициент прохождения для потенциала из задачи 2.9 в квазиклассическом приближении дается этой формулой.

ЗАДАЧА 6.2 (ОТРАЖЕНИЕ НАД БАРЬЕРОМ). ПредПоЛОЖИМ, что Потенциал $V(x)$ допускает аналитическое продолжение в верхнюю полуплоскость, и пусть E - энергия, такая, что $E > V(x)$ для всех вещественных x. Предположим, что существует лишь одно комплексное x_0, такое, что $V(x_0) = E$. Покажите, что в квазиклассическом приближении

$$R_{\text{WKB}} = e^{-\frac{4}{\hbar}\operatorname{Im}\int\limits_a^{x_0} p(x)dx}$$

где $p(x) = \sqrt{2m(E - V(x))}$, а $a \in \mathbb{R}$ (выбор a не влияет на мнимую часть интеграла в экспоненте). Проверьте непосредственно, что коэффициент отражения для потенциала в задаче 2.9 в квазиклассическом приближении дается этой формулой.

ЗАДАЧА 6.3. Найдите коэффициенты прохождения и отражения для параболического барьера - потенциала $V(x) = -\frac{1}{2}kx^2$, где $k > 0$, - и проверьте непосредственно, что в квазиклассическом приближении они удовлетворяют при $E < 0$ и $E > 0$ соответственно формулам из задач 6.1 и 6.2.

6.9.7 Bohr-Wilson-Sommerfeld Quantization Rules

(combine with some sections before and move partially it to a section before!!)

Метод ВКБ позволяет определить уровни энергии в квазиклассическом приближении. Рассмотрим для простоты финитное движение одномерной частицы в потенциальной яме: в потенциале $V(x)$ с энергией E, такое, что имеются две точки поворота a и b. Классическая область - это $a \leqslant x \leqslant b$, и движение периодично с периодом

$$T = 2\int\limits_a^b \frac{dx}{\dot{x}} = 2m\int\limits_a^b \frac{dx}{p} = \sqrt{2m}\int\limits_a^b \frac{dx}{\sqrt{E - V(x)}}$$

Области $x < a$ и $x > b$ недоступны (см. раздел 1.1.5 главы 1). Из (6.21) - (6.22) следует, что волновая функция ВКБ экспоненциально затухает в недоступных областях $x < a$ и $x > b$. Воспользовавшись (6.21), мы видим, что в классической области волновая функция ВКБ имеет вид

$$\psi_{\text{wKB}}(x) = \frac{2A}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int\limits_a^x p(s)ds + \frac{\pi}{4}\right)$$

тогда как, используя (6.22), получаем

$$\begin{aligned}\psi_{\text{WKB}}(x) &= \frac{2B}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int\limits_x^b p(s)ds + \frac{\pi}{4}\right) = \\ &= \frac{2B}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int\limits_a^b p(s)ds + \frac{\pi}{2} - \left(\frac{1}{\hbar}\int\limits_a^x p(s)ds + \frac{\pi}{4}\right)\right).\end{aligned}$$

Эти два выражения определяют одну и ту же функцию на $a \leqslant x \leqslant b$, если и только если существует положительное целое число n, такое, что

$$\frac{1}{\hbar}\int\limits_a^b p(x)dx + \frac{\pi}{2} = (n+1)\pi$$

тогда $A = (-1)^{n+1}B$. Уравнение (6.23), записанное в виде

$$1.\quad \int\limits_a^b \sqrt{2m(E - V(x))}dx = \pi\hbar\left(n + \frac{1}{2}\right),$$

определяет квазиклассические уровни энергии. Из (6.21) - (6.22) следует, что число n равно количеству нулей волновой функции ВКБ. В соответствии с теоремой об осцилляции случай $n = 0$ отвечает основному состоянию, случай $n = 1$ - состоянию со следующим уровнем энергии, и т. д. Обозначив, как и в главах 1 и 2, координату x как q, можно переписать (6.23) как

$$\oint p dq = 2\pi\hbar\left(n + \frac{1}{2}\right)$$

где интегрирование идет по замкнутой классической орбите в фазовой плоскости $\mathbb{R}^2$ с каноническими координатами p, q. Условие (6.24) - это известное правило квантования Бора - Вильсона - Зоммерфельда для случая одной степени свободы (см. раздел 2.2.5

главы 2). Подчеркнем, что, вообще говоря, правило квантования БВЗ применимо только для больших n и дает квазиклассическую асимптотику уровней энергии E_n. Однако, как было показано в разделе 2.2.6 главы 2, уровни энергии гармонического осциллятора, полученные по правилу БВЗ, точны. Правила БВЗ также точны для уровней энергии атома водорода (см. раздел 3.5.1).

Этот квазиклассический анализ можно обобщить на системы с n степенями свободы, соответствующие вполне интегрируемым классическим гамильтоновым системам (см. раздел 1.2.6 главы 1). Правила квантования Бора- Вильсона - Зоммерфельда принимают вид

$$\oint_\gamma \boldsymbol{p} d\boldsymbol{q} = 2\pi\hbar \left(\boldsymbol{n}_\gamma + \frac{1}{4} \operatorname{ind} \gamma \right).$$

Здесь интегрирование ведется по всем 1-циклам γ в лагранжевом подмногообразии $\Lambda = \{(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{R}^{2n} : H_c(\boldsymbol{p}, \boldsymbol{q}) = E, F_2(\boldsymbol{p}, \boldsymbol{q}) = E_2, ..., F_n(\boldsymbol{p}, \boldsymbol{q}) = \ = E_n\}$, a ind γ - индекс Маслова цикла γ в Λ. Для переменных действие-угол (I, φ) интегрирование в (6.25) ведется по базисным 1циклам n-тора T^n, и получаются условия квантования $I_i = \left(n_i + \frac{1}{2}\right)\hbar$, $i = 1, ..., n$.

6.9.8 Other About Semiclassics

(тут интересные дополнительные вопросы)

связь квантовой механики и оптики

(оставленный вопрос, потом подумаю.)

Метод transfer-matrix по Киселеву

(перенес сюда, потому что вряд ли это нужно)

Суть по Киселеву (???)

При наличии нескольких потенциальных ям и потенциальных барьеров применяют технику transfer-matrix. Эта техника описывает линейные преобразования для коэффициентов в суперпозиции квазиклассических решений стационарного уравнения Шрёдингера. Пусть строка

$$\left(C_-^\uparrow, C_-^\downarrow\right)$$

отвечает суперпозиции решений

$$\frac{C_-^\uparrow}{\sqrt{|p(x)|}} \mathrm{e}^{\frac{1}{\hbar}\int\limits_a^x |p(x)|\mathrm{d}x} + \frac{C_-^\downarrow}{\sqrt{|p(x)|}} \mathrm{e}^{-\frac{1}{\hbar}\int\limits_a^x |p(x)|\mathrm{d}x}$$

в области $-\infty < x < a$, где a - координата точки поворота, значение которой меньше значений всех координат других точек поворота. Ясно, что коэффициент $C_-^\uparrow$ отвечает решению, которое растет при увеличении x, а $C_-^\downarrow$ решению, которое убывает с увеличением x. Выше мы рассмотрели случай сшивки решения возле точки поворота при $C_-^\downarrow = 0$ и при $x > a$ пришли к решению

$$\frac{C_-^\dagger}{\sqrt{|p(x)|}} \left(\mathrm{e}^{\frac{i}{\hbar}\int\limits_a^x |p(x)|\mathrm{d}x - \mathrm{i}\frac{\pi}{4}} + \mathrm{e}^{-\frac{i}{\hbar}\int\limits_\alpha^x |p(x)|\mathrm{d}x + \mathrm{i}\frac{\pi}{4}} \right)$$

которое можно представить как строку, составленную из коэффициентов для волн, которые распространяются по оси x и против оси x, соответственно

$$\left(C_-^{\uparrow}\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}\mathrm{e}^{\frac{i}{\hbar}S(x,a)}, C_-^{\uparrow}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}\mathrm{e}^{-\frac{1}{\hbar}S(x,a)}\right),$$

где действие

$$S(x,a)=\int\limits_a^x |p(x)|\mathrm{d}x.$$

Если бы при $x<a$ мы точно также рассмотрели решение, которое убывает с ростом x, т.е. решение с $C_-^{\uparrow}=0$, что отвечает только смене знака аргумента в экспоненте, как видно из (12.48), то получили бы решение

$$\frac{C_-^{\downarrow}}{\sqrt{|p(x)|}}\left(\mathrm{e}^{-\frac{i}{\hbar}\int\limits_a^x |p(x)|\mathrm{d}x-\mathrm{i}\frac{\pi}{4}}+\mathrm{e}^{\frac{i}{\hbar}\int\limits_a^x |p(x)|\mathrm{d}x+\mathrm{i}\frac{\pi}{4}}\right),$$

которое можно представить как строку, составленную из коэффициентов для волн, которые распространяются по оси x и против оси x, соответственно

$$\left(C_-^{\downarrow}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}\mathrm{e}^{\frac{1}{\hbar}S(x,a)}, C_-^{\downarrow}\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}\mathrm{e}^{-\frac{i}{\hbar}S(x,a)}\right).$$

В методе transfer-matrix эти линейные преобразования со строками из коэффициентов решений из области $x<a$ слева от точки поворота в область $x>a$ справа от точки поворота представляют сначала как произведение строки на матрицу фазовых сдвигов в точке поворота,

$$T(a)=\begin{pmatrix} \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}} & \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} \\ \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} & \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}} \end{pmatrix}$$

в которой первая строка отвечает фазовым сдвигам для решения (12.50), а вторая - (12.53). Затем происходит распространение от точки поворота a до точки $x>a$, что отвечает умножению на диагональную матрицу

$$T(x,a)=\begin{pmatrix} \mathrm{e}^{\frac{1}{\hbar}S(x,a)} & 0 \\ 0 & \mathrm{e}^{-\frac{i}{\hbar}S(x,a)} \end{pmatrix}$$

так что матричное умножение

$$\left(C_-^{\uparrow}, C_-^{\downarrow}\right)\circ T(a)\circ T(x,a)$$

выдает строку, которая в точности воспроизводит оба результата (12.50) и (12.53) одновременно 1.

Универсальность метода transfer-matrix заключается в том, что матрица фазовых сдвигов $T(a)$ не зависит от того, с какой стороны от точки поворота расположена область, доступная для классической частицы! В самом деле, если мы теперь рассмотрим точку поворота b, для которой область, не доступная для классической частицы, расположена при $x>b$, то в этой области суперпозиция растущего при увеличении x решения и убывающего решения

$$\frac{C_+^{\uparrow}}{\sqrt{|p(x)|}}\mathrm{e}^{\frac{1}{\hbar}\int\limits_b^x |p(x)|\mathrm{d}x}+\frac{C_+^{\downarrow}}{\sqrt{|p(x)|}}\mathrm{e}^{-\frac{1}{\pi}\int\limits_b^x |p(x)|\mathrm{d}x}$$

можно представить в виде столбца

$$\begin{pmatrix} C_+^{\uparrow} \\ C_+^{\downarrow} \end{pmatrix}$$

так что после умножения слева на ту же матрицу фазовых сдвигов мы получим

$$T(b) \circ \begin{pmatrix} C_+^{\uparrow} \\ C_+^{\downarrow} \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}} C_+^{\uparrow} + \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} C_+^{\downarrow} \\ \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} C_+^{\uparrow} + \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}} C_+^{\downarrow} \end{pmatrix}$$

При $C_+^{\uparrow} = 0$, когда при $x > b$ есть только убывающее на бесконечности решение, это соответствует тому, что падающая на потенциальный барьер волна (верхняя позиция в столбце) опережает отраженную волну (нижняя позиция в столбце) на $\pi/2$, как это и должно быть. Затем решение в точке $x < b$ получается умножением на диагоналную матрицу распространения от точки поворота b до точки $x : T(x, b)$.

Если между потенциальными ямами встречается потенциальный барьер и $p^2 < 0$, то в матрице распространения необходимо провести подстановку: вместо вещественного действия для распространяющейся по оси x волны нужно получить растущую с увеличением x экспоненту, а значит, обобпение (12.51) имеет вид $S(x,a) = \int\limits_a^x |p(x)|\mathrm{d}x, \quad p^2(x) > 0, \; S(x,a) = -\mathrm{i}\int\limits_a^x |p(x)|\mathrm{d}x, \quad p^2(x) < 0.$ Итак, метод линейных преобразований с матрицами фазовых сдвигов и матрицами распространения позволят чисто алгебраически получать квазиклассическое решение в любой области, как доступной, так и не доступной для классической частицы, если при заданной энергии у потенциала есть несколько точек поворота и несколько потенциальных барьеров.

О применениях (???)

(пока хз)

Einstein–Brillouin–Keller method (??)

(вики. пока не актуально, но не знал, что такое есть.)

The Einstein-Brillouin-Keller method (EBK) is a semiclassical method (named after Albert Einstein, Léon Brillouin, and Joseph B. Keller) used to compute eigenvalues in quantum-mechanical systems. EBK quantization is an improvement from Bohr-Sommerfeld quantization which did not consider the caustic phase jumps at classical turning points. [1] This procedure is able to reproduce exactly the spectrum of the 3D harmonic oscillator, particle in a box, and even the relativistic fine structure of the hydrogen atom. [2]

In 1976-1977, Michael Berry and M. Tabor derived an extension to Gutzwiller trace formula for the density of states of an integrable system starting from EBK quantization. [3][4] There have been a number of recent results on computational issues related to this topic, for example, the work of Eric J. Heller and Emmanuel David Tannenbaum using a partial differential equation gradient descent approach. [5]

Given a separable classical system defined by coordinates $(q_i, p_i)\,; i \in \{1, 2, \cdots, d\}$, in which every pair (q_i, p_i) describes a closed function or a periodic function in q_i, the EBK procedure involves quantizing the line integrals of p_i over the closed orbit of q_i:

$$I_i = \frac{1}{2\pi} \oint p_i dq_i = \hbar \left(n_i + \frac{\mu_i}{4} + \frac{b_i}{2} \right)$$

where I_i is the action-angle coordinate, n_i is a positive integer, and μ_i and b_i are Maslov indexes. μ_i corresponds to the number of classical turning points in the trajectory of q_i (Dirichlet boundary condition), and b_i corresponds to the number of reflections with a hard wall (Neumann boundary condition). [6]

7 Methods for Scatterings

7.1 Green's Function Methods (??)

(разедл оставлен, потому что пока что не дошел до него,. потом мб большим сделаю)

7.1.1 Idea of GF Method

Суть (?)

Функция Грина в квантовой механике

Основным объектом диаграммной техники является функция Грина. Она определяется через ψ -операторы, взятые в представлении взаимодействия:

$$\tilde{\psi}_\alpha(x) = e^{i\widehat{\mathcal{H}}_0 t}\widehat{\psi}_\alpha(\mathbf{r})e^{-i\widehat{\mathcal{H}}_0 t},$$
$$\tilde{\psi}^+_\alpha(x) = e^{i\widehat{\mathcal{H}}_0 t}\widehat{\psi}^+_\alpha(\mathbf{r})e^{-i\widehat{\mathcal{H}}_0 t}$$

где под x понимается совокупность четырех переменных - координат $\mathbf{r}$ и времени t; α -спиновый индекс (для фермионов).

Так называемая причинная функция Грина есть среднее от хронологического произведения ψ -операторов, взятых в представлении взаимодействия:

$$G^c_{\alpha\beta}(x,x') = -i\left\langle \mathrm{T}\tilde{\psi}_\alpha(x)\tilde{\psi}^+_\beta(x')\right\rangle$$

где скобки $\langle ... \ \rangle$ означают матричный элемент $\left\langle \widehat{S}_0\right\rangle^{-1}\langle 0|...|0\rangle$, взятый по основному состоянию системы с гамильтонианом $\widehat{\mathcal{H}}_0$. (Фазовый множитель $\left\langle \widehat{S}_0\right\rangle = \left\langle 0\left|e^{-i\widehat{\mathcal{H}}_0 t}\right|0\right\rangle_{t\to\infty}$ принято вводить для нормировки.)

Таким образом, функции Грина бозонов и фермионов определяются одинаково, но операция Т-упорядочения имеет разный смысл.

В выражении (2.7) и всюду далее там, где это не приводит к недоразумениям, мы используем систему единиц, в которой $\hbar = 1, [t] = [E]^{-1}$. Кроме того, мы также часто будем писать ψ вместо $\tilde{\psi}$, ибо основную роль в диаграммной технике играет именно операторы $\tilde{\psi}$ в представлении взаимодействия, а операторы ψ в шредингеровском представлении практически не встречаются. В однородной системе (скажем, в газе или в жидкости) функция Грина (2.8), очевидно, зависит только от разности координат $\mathbf{r}-\mathbf{r}'$ и времен $t-t'$. В этом случае удобно сделать преобразование Фурье и перейти в импульсно-частотное представление

$$G_{\alpha\beta}(x-x') = \iint G_{\alpha\beta}(\varepsilon,\mathbf{p})e^{-i\varepsilon(t-t')+i\mathbf{p}(\mathbf{r}-\mathbf{r}')}\frac{d\varepsilon d^3p}{(2\pi)^4}$$

В этом представлении обычно и строится диаграммная техника.

О способах поиска (???)

$G_{\alpha\beta}(\varepsilon,\mathbf{p})$ для идеального газа находится, пользуясь определением $G^c_{\alpha\beta}(x,x') = -i\left\langle \mathrm{T}\tilde{\psi}_\alpha(x)\tilde{\psi}^+_\beta(x')\right\rangle$.

Примеры функций Грина

Например, для идеального ферми-газа она имеет вид

$$G_{\alpha\beta}(\varepsilon, \mathbf{p}) = \frac{\delta_{\alpha\beta}}{\varepsilon - \xi(\mathbf{p}) + i0\,\mathrm{sign}\,(|\mathbf{p}| - p_0)}$$

где $\xi(\mathbf{p}) = \mathbf{p}^2/2m - E_F$ -закон дисперсии, а $p_0 = \sqrt{2mE_F}$ -импульс Ферми, являющийся границей распределения ферми-частиц по импульсам.

Величины по функции Грина (!?!?!)

(добавлю сюда то, что еще не написано!!!)
Приведем вид различных физических величин через функцию Грина.

одночастичная матрица плотности

$$\rho_{\alpha\beta}\,(\mathbf{r}, \mathbf{r}', t) = \pm i \lim_{t' \to t+0} G_{\alpha\beta}\,(x, x')$$

где знак соответствует статистике: «+»для бозонов, «-» для фермионов.
(?? почему)

плотность частиц

Зная $\rho_{\alpha\beta}\,(\mathbf{r}, \mathbf{r}', t)$, нетрудно найти среднее любой величины. Например, плотность частиц выражается через функцию Грина как

$$n(x) = \pm i \lim_{t' \to t+0} \mathrm{Tr}\, G_{\alpha\beta}\,(x, x')$$

плотность тока

Плотность тока есть

$$\mathbf{j}(x) = \pm \frac{\hbar}{2m} \lim_{\substack{t' \to t+0 \\ \mathbf{r}' \to \mathbf{r}}} (\nabla_{\mathbf{r}} - \nabla_{\mathbf{r}'})\, \mathrm{Tr}\, G_{\alpha\beta}\,(x, x')$$

где Tr обозначает взятие следа по спиновым индексам α, β. Брать предел по $t' > t$ в соотношениях (2.11) – (2.13) необходимо из-за неоднозначности определения функции Грина при $t = t'$.

Пример, когда без T-упорядочения происходят неверные расчеты

(вопрос остался, потом подумаю, пока влом.)

Типичные примеры (?)

Как догадаться про это?

Equvalence of the definitions of GFs

First, the term "propagator" is usually defined as the Green's function of the first type, not the second type, i.e. as a solution to the diffential equation $\hat{L}G = \delta$.

At any rate, those definitions are ultimately equivalent – when the details are correctly written down – because the Green's function defined as the correlator in the second definition obeys the first differential equation.

The differential operator $\hat{L}$ is what appears in the linearized equations of motion for the field, in this case $\psi(x_1, t_1)$, and it only acts on $\psi(x_1, t_1)$, not $\psi^\dagger(x_2, t_2)$.

The time-ordering operator T may be written in terms of the step function

$$T(\psi\psi^\dagger) = \psi\psi^\dagger \cdot \theta(t_1 - t_2) - \psi^\dagger\psi \cdot \theta(-t_1 + t_2)$$

where ψ is always at x_1, t_1 and $\psi^\dagger$ is at x_2, t_2. Now, ask what happens when you act with $\hat{L}$ on the right hand side of the displayed equation above.

By the Leibniz rule, there are the terms with $\hat{L}\psi = 0$. It vanishes by the equations of motion. But there are extra terms where $\hat{L}$ acts on the step functions.

The operator $\hat{L}$ contains the term that differentiates with respect to t_1 multiplied by a coefficient C. This turns $\theta(t_1 - t_2)$ to $\delta(t_1 - t_2)$. The same occurs in the next term, but with the opposite sign which cancels the sign that was already there. So the extra terms are

$$\hat{L}T(\psi\psi^\dagger) = C\delta(t_1 - t_2)(\psi\psi^\dagger + \psi^\dagger\psi)$$

I got two terms because there were two terms. However, these two terms exactly combine to the anticommutator of ψ and $\psi^\dagger$ which only needs to be evaluated for $t_1 = t_2$, the equal-time anticommutator, and the result is $D \cdot \delta(x_1 - x_2)$.

That's why the action of $\hat{L}$ on the correlator ends up being $CD\delta(t_1 - t_2)\delta(x_1 - x_2)$ where the constants C, D are mostly just factors of i etc.

For bosonic fields, $\hat{L}$ has the second derivative with respect to time. One of the derivatives has the fate as above, the other one turns the other ϕ, which plays the role of $\psi^\dagger$, into $\partial_t\phi$ which is the canonical momentum, and it's the right variable that has the δ-function-like commutator. Also, the intermediate sign is the opposite one but the result is the same, some $CD \cdot \delta \cdot \delta$.

from https://physics.stackexchange.com/questions/201482/two-definitions-of-greens-function

(допишу лучше!! про усреднение прокомментриую всё!)

7.1.2 Why GF Method is That Powerful?

(overview of applications and explanation why it works?)

7.1.3 GF Method for Time-Dependent Problems?

(main subsubsection about it, maybe later I'll create a few of them)

7.1.4 GF Method for Matrix Hamiltonians

(I'll prepare something about matrix inversions, like for that problem in theorminimum. a useful preparation)

7.2 Scattering Theory: Perturbative Approach

7.2.1 Concept of Scattering Cross-Section

Что такое сечение рассеяния?

(см. Тонга, общий бэкграунд, потом напишу, пока в механике об этом писал)

Особенности сечений рассеяния

Примеры сечений

(соберу графики, чтобы представлять, что в итоге моделей)

Что если сечение расходится?

(это не редкая ситуация, ибо даже сечение рассяния на потенциале $1/r^2$ в 3д расходится. допишу потом, как это понимать???)

Пока ответ в том, что считаем просто дифференциальное и всё.

7.2.2 Spherical Waves of a Free Particle

Сферические волны по Киселеву

Уравнение для стационарного состояния с энергией $E(k) = \frac{\hbar^2 k^2}{2m}$ и заданным значением орбитального момента l и его проекции m

$$\psi(\boldsymbol{r}) = R_{kl}(r)Y_{l,m}(\theta, \phi)$$

в области, где потенциал мал, есть

$$R''_{kl}(r) + \frac{2}{r}R'_{kl}(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right)R_{kl}(r) = 0$$

т.е. является уравнением для свободной частицы, которое мы и исследуем более детально В этом параграфе.

Согласно общему свойству радиального уравнения при $r \to 0$

$$R_{kl}(r) \sim r^l$$

так что проведем замену функции

$$R_{kl}(r) = r^l \chi_{kl}(r)$$

При ней $R'_{kl}(r) = r^l\chi'_{kl} + lr^{l-1}\chi_{kl}$, $R''_{kl}(r) = r^l\chi''_{kl} + 2lr^{l-1}\chi'_{kl} + l(l-1)r^{l-2}\chi_{kl}$. Подставим, придем к

$$\chi''_{kl} + \frac{2}{r}(l+1)\chi'_{kl} + k^2\chi_{kl} = 0$$

Введем

$$\chi_{kl}(r) = v_{kl}(z), \quad z = r^2$$

При ней $\chi'_{kl} = 2rv'_{kl}$, $\chi''_{kl} = 4zv''_{kl} + 2v'_{kl}$. Получим

$$4zv''_{kl} + 2(2l+3)v'_{kl} + k^2 v_{kl} = 0$$

Продифференцируем:

$$4zv'''_{kl} + 2(2(l+1)+3)v''_{kl} + k^2 v'_{kl} = 0$$

Это уравнение тождественно удовлетворяется, если v'_{kl} является решением уравнения Для $v_{k(l+1)}$, т. е.

$$v_{k(l+1)}(z) = Bv'_{kl}(z) \to \chi_{k(l+1)}(r) = \frac{B}{2r}\chi'_{kl}(r)$$

Положим $B = 2$ и запишем выведенные нами рекуррентные соотношения для радиальных волновых функций с различными значениями орбитального момента в виде

$$R_{kl}(r) = c_l \frac{r^l}{k^l} \left(\frac{1}{r} \frac{d}{dr} \right)^l R_{k0}(r)$$

Здесь $R_{k0}(r)$ -решение радиального уравнения для $l = 0$, фактор k^{-l} введен для удобства, аc_l -нормировочные постоянные.

Для $R_{k0}(r) = u(r)/r$ стандартно имеем

$$u'' + k^2 u = 0$$

откуда ясно, что функция $u(r)$ представима в виде суперпозиции двух независимых решений

$$u = \tilde{c}_0 \left\{ -e^{-\mathrm{i}kr} + S_0 e^{\mathrm{i}kr} \right\}$$

или

$$R_{k0}(r) = \frac{\tilde{c}_0}{r} \left\{ -e^{-\mathrm{i}kr} + S_0 e^{\mathrm{i}kr} \right\}$$

где S_0 -константа относительной нормировки расходящейся части волны.

Полагая $\tilde{c}_0 =$ потенциал обращается в нуль, и в частности, в асимптотической области $r \to \infty$

$$R_{kl}(r) = c_l \frac{r^l}{k^l} \left(\frac{1}{r} \frac{d}{dr} \right)^l \frac{1}{r} \left\{ -e^{-\mathrm{i}kr} + S_l e^{\mathrm{i}kr} \right\}$$

При $r \to \infty$ ведущий вклад получается дифференцированием экспонент, так что

$$\begin{aligned} R_{kl}(r) &\simeq c_l \frac{\mathrm{i}^l}{r} \left\{ (-1)^{l+1} e^{-\mathrm{i}kr} + S_l e^{\mathrm{i}kr} \right\} \\ &= c_l \frac{(-1)^l}{r} \left\{ -e^{-\mathrm{i}\left(kr - \frac{\pi}{2} l\right)} + S_l e^{\mathrm{i}\left(kr - \frac{\pi}{2} l\right)} \right\} \end{aligned}$$

Если потенциал тождественно равен нулю, то уравнение справедливо во всем пространстве, и приведенное общее выражение необходимо ограничить на случай свободной частицы: волновая функция должна вести себя как r^l при $r \to 0$. Экспоненты в радиальной функции общего вида (13.9) можно разложить в сумму синуса и косинуса от kr, из разложения которых в ряд Тейлора сразу следует, что вклад косинуса необходимо занулить, так как он приводит к члену $1/r$, дифференцирование которого дает сингулярность при $r = 0$ Напротив, для вклада синуса получим

$$\left(\frac{1}{r} \frac{d}{dr} \right)^l \frac{\sin kr}{r} \bigg|_{r \to 0} = (-1)^l \left(\frac{1}{r} \frac{d}{dr} \right)^l \frac{(kr)^{2l+1}}{r(2l+1)!} \bigg|_{r \to 0} = (-1)^l k^{2l+1} \frac{(2l)!!}{(2l+1)!}$$

так что радиальная волновая функция имеет правильное поведение в нуле.

Итак, для этого необходимо, чтобы для свободной частицы

$$S_l^{(0)} \equiv 1$$

и тогда

$$R_{kl}^{(0)}(r) = c_l^{(0)} (-1)^l \frac{r^l}{k^l} \left(\frac{1}{r} \frac{d}{dr} \right)^l \frac{1}{r} \left\{ -e^{-\mathrm{i}kr} + e^{\mathrm{i}kr} \right\}$$

что в асимптотической области $r \to \infty$ дает

$$\begin{aligned} R_{kl}^{(0)}(r) &\simeq c_l^{(0)} \frac{1}{r} \left\{ -e^{-\mathrm{i}\left(kr - \frac{\pi}{2} l\right)} + e^{\mathrm{i}\left(kr - \frac{\pi}{2} l\right)} \right\} \\ &= c_l^{(0)} \frac{2\mathrm{i}}{r} \sin\left(kr - \frac{\pi}{2} l \right) \end{aligned}$$

Для центрального потенциала, достаточно быстро обращающегося в нуль на бесконечности, радиальная волновая функция общего вида (13.9) в задаче рассеяния описывает в асимптотической области суперпозицию падающей на мишень и рассеянной волн со сферическим фронтом (27.10). В силу унитарности падающий и рассеянный потоки равны друг другу для упругого рассеяния, т. е.

$$|S_l| \equiv 1, \quad S_l = \mathrm{e}^{2\mathrm{i}\delta_l}, \quad \delta_l \in \mathbb{R},$$

где δ_l - фазовые сдвиги, зависящие от потенциала, энергии и орбитального момента. По построению

$$\delta_l \in [0, \pi]$$

Значит, при $r \to \infty$ волновая функция в разложении по парциальным волнам имеет вид

$$\begin{aligned} R_{kl}(r) &\simeq c_l^{(0)} \frac{1}{r} \left\{ -e^{-\mathrm{i}\left(kr - \frac{\pi}{2}l\right)} + S_l e^{\mathrm{i}\left(kr - \frac{\pi}{2}l\right)} \right\} \\ &= c_l^{(0)} \frac{2\mathrm{i}}{r} e^{\mathrm{i}\delta_l} \sin\left(kr - \frac{\pi}{2}l + \delta_l\right) \end{aligned}$$

Подчеркнем, что в этой формуле коэффициенты $C_l^{(0)}$ те же, что и в разложении по парциальным волнам волновой функции свободной частицы, так как в задаче рассеяния падающая волна В стационарном out-состоянии должна тождественно совпадать в падающей волной свободного in-состояния.

Итак, мы установили, что в случае исключительно упругих столкновений процесс рассеяния описывается парциальными фазовым и сдвигами, и определили асимптотический вид волновой функции в задаче рассеяния.

Теперь для расчета сечения необходимо отнормировать парциальные потоки так, Чтобы они отвечали потокам падающей волны де Бройля, потому что в эксперименте осуществляется только такая возможность, когда состояниями асимптоти ческого in-пространства являются именно свободные монохроматические волны, а для out-состояний возможен парциально-волновой анализ: наблюдается разложение по орбиталям.

7.2.3 Expansion of the de Broglie Wave into Partial Waves

Разложение волны де Бройля по парциальным волнам по Киселеву

Разложим состояние $|\boldsymbol{k}\rangle$ с заданным волновым вектором $\boldsymbol{k}$ по базису свободных сферических волн $|k; l, m\rangle$ с энергией $E = \hbar^2 k^2/2m$ и орбитальным моментом l с проекцией m в координатном пространстве:

$$\langle \boldsymbol{r}|\boldsymbol{k}\rangle = \sum_{l,m} \langle \boldsymbol{r}|k; l, m\rangle \langle k; l, m|\boldsymbol{k}\rangle$$

Обычно вводят единичные векторы

$$\boldsymbol{n} = \frac{\boldsymbol{r}}{r}, \quad \boldsymbol{n}^{(k)} = \frac{\boldsymbol{k}}{k}$$

Тогда, очевидно, волна де Бройля

$$\langle \boldsymbol{r}|\boldsymbol{k}\rangle = e^{\mathrm{i}kr\boldsymbol{n}\cdot\boldsymbol{n}^{(k)}}$$

Состояние $\langle \boldsymbol{r}|k; l, m\rangle$ есть ничто иное, как решение стационарного уравнения Шредингера для свободной частицы в координатном представлении

$$\langle \boldsymbol{r}|k; l, m\rangle = R_{kl}(r) Y_{l,m}(\boldsymbol{n})$$

где $Y_{l,m}(\boldsymbol{n})$ - сферическая гармоника, которая зависит от угловых координат единичного радиус-вектора $\boldsymbol{n}$, а $\langle k; l, m|\boldsymbol{k}\rangle$ - эрмитово сопряженное решение стационарного уравнения Шредингера в импульсном представлении (представлении волнового вектора):

$$\langle k; l, m|\boldsymbol{k}\rangle = \tilde{R}^*_{kl}(k) Y^*_{l,m}\left(\boldsymbol{n}^{(k)}\right)$$

Переопредели м радиальную волновую функцию, поглощая фактор $\widetilde{R}_{kl}(k)$, так что в согласии с общим рассмотрением свободных сферических волн разложение примет вид

$$e^{\mathrm{i}kr\boldsymbol{n}\cdot\boldsymbol{n}^{(k)}} = 4\pi \sum_{l,m} R^{(0)}_{kl}(r) Y_{l,m}(\boldsymbol{n}) Y^*_{l,m}\left(\boldsymbol{n}^{(k)}\right)$$

где

$$R^{(0)}_{kl}(r) = c^{(0)}_l (-1)^l \frac{r^l}{k^l} \left(\frac{1}{r}\frac{d}{dr}\right)^l \frac{1}{r}\left\{-e^{-\mathrm{i}kr} + e^{\mathrm{i}kr}\right\}$$

с неизвестными коэффициентами $c^{(0)}_l$, задачу определения которых мы сейчас решаем.

В волне скалярное произведение векторов $\boldsymbol{n}\cdot\boldsymbol{n}^{(k)}$ симметрично по перестановке единичных векторов, в разложении же стоит произведение сферических гармоник $Y_{l,m}(\boldsymbol{n})Y^*_{l,m}\left(\boldsymbol{n}^{(k)}\right)$, которое можно преобразовать, пользуясь свойством комплексного сопряжения сферических функций

$$Y_{l,m}(\boldsymbol{n}) = (-1)^m Y^*_{l,-m}(\boldsymbol{n})$$

откуда

$$Y_{l,m}(\boldsymbol{n}) Y^*_{l,m}\left(\boldsymbol{n}^{(k)}\right) = Y^*_{l,-m}(\boldsymbol{n}) Y_{l,-m}\left(\boldsymbol{n}^{(k)}\right)$$

и значит, суммирование по m в правой части разложения (13.19) дает результат, симметричный по перестановке единичных векторов, как это и должно быть.

Вычислим коэффициенты разложения $C^{(0)}_l$ в случае, когда волновой вектор направлен вдоль оси z, откуда $\boldsymbol{n}\cdot\boldsymbol{n}^{(k)} = \cos\theta$, т.е. $\theta^{(k)} = \phi^{(k)} = 0$, и в разложении участвуют только вклады с $m = 0$

$$Y^*_{l,m}\left(\boldsymbol{n}^{(k)}\right) \mapsto Y^*_{l,0}(0,0) = \sqrt{\frac{2l+1}{4\pi}} P_l(1) = \sqrt{\frac{2l+1}{4\pi}}$$

$$Y_{l,m}(\boldsymbol{n}) \mapsto Y_{l,0}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)$$

Тогда разложение принимает вид

$$e^{\mathrm{i}kr\cos\theta} = \sum_l (2l+1) P_l(\cos\theta) R^{(0)}_{kl}(r)$$

Из ортогональности полиномов Лежандра

$$\int_{-1}^{1} d\cos\theta \cdot P_{l'}(\cos\theta) P_l(\cos\theta) = \frac{2}{2l+1}\delta_{ll'}$$

и принятого разложения следует, что

$$\int_{-1}^{1} d\cos\theta \cdot P_l(\cos\theta) e^{\mathrm{i}kr\cos\theta} = 2R^{(0)}_{kl}(r).$$

Рассмотрим обе части этого равенства при $r \to \infty$. Слева интегрирование по частям дает

$$\int\limits_{-1}^{1} d\cos\theta \cdot P_l(\cos\theta) e^{\mathrm{i}kr\cos\theta} = \frac{1}{\mathrm{i}kr} P_l(\cos\theta) e^{\mathrm{i}kr\cos\theta|^{+1}_{-1}} - \frac{1}{\mathrm{i}kr} \int\limits_{-1}^{1} d\cos\theta \cdot P_l'(\cos\theta) e^{\mathrm{i}kr\cos\theta}$$

Интегрирование по частям следует повторить еще $l-1$ раз, так как полином Лежандра P_l является полиномом степени l. Однако в пределе $r \to \infty$ каждый дополнительный шаг интегрирования по частям приводит к вкладам $\mathcal{O}\left(1/r^2\right)$. Таким образом,

$$\int\limits_{-1}^{1} d\cos\theta \cdot P_l(\cos\theta) e^{\mathrm{i}kr\cos\theta} = \frac{1}{\mathrm{i}kr} P_l(\cos\theta) e^{\mathrm{i}kr\cos\theta}\Big|_{-1}^{+1} + \mathcal{O}\left(\frac{1}{r^2}\right)$$

По построению $P_l(1) = 1$ и $P_l(-1) = (-1)^l$, так что окончательно асимптотически получаем

$$\int\limits_{-1}^{1} d\cos\theta \cdot P_l(\cos\theta) e^{\mathrm{i}kr\cos\theta} \simeq \frac{1}{\mathrm{i}kr} \left\{ e^{\mathrm{i}kr} - (-1)^l e^{-\mathrm{i}kr} \right\}$$

С другой стороны, асимптотическое поведение радиальной волновой функции сферической волны было нами установлено в предыдущем параграфе

$$R_{kl}^{(0)}(r) \simeq c_l^{(0)} (-\mathrm{i})^l \frac{1}{r} \left\{ e^{\mathrm{i}kr} - (-1)^l e^{-\mathrm{i}kr} \right\}$$

Значит, из (13.21) находим

$$c_l^{(0)} = \mathrm{i}^l \frac{1}{2\mathrm{i}k}$$

Таким образом, разложение окончательно принимает вид

$$e^{\mathrm{i}kr\cos\theta} = \sum_l (2l+1) P_l(\cos\theta) (-\mathrm{i})^l \frac{r^l}{2\mathrm{i}k^{l+1}} \left(\frac{1}{r}\frac{d}{dr} \right)^l \frac{1}{r} \left\{ -e^{-\mathrm{i}kr} + e^{\mathrm{i}kr} \right\}$$

с асимптотикой при $r \to \infty$

$$\begin{aligned} e^{\mathrm{i}kr\cos\theta} &\simeq \sum_l (2l+1) P_l(\cos\theta) \frac{1}{2\mathrm{i}kr} \left\{ e^{\mathrm{i}kr} - (-1)^l e^{-\mathrm{i}kr} \right\} \\ &= \sum_l (2l+1) P_l(\cos\theta) \mathrm{i}^l \cdot \frac{\sin\left(kr - \frac{\pi}{2}l\right)}{kr} \end{aligned}$$

7.2.4 Born Approximation

Теория

В ведущем приближении итераций в уравнении для $\mathcal{T}_E$-матрицы или, что то же, в интегральном уравнении для волновой функции рассеяния

$$\mathcal{T}_E \approx V, \quad \langle \boldsymbol{k}_\mathrm{f} | \mathcal{T}_E | \boldsymbol{k}_\mathrm{i} \rangle \approx \langle \boldsymbol{k}_\mathrm{f} | V | \boldsymbol{k}_\mathrm{i} \rangle ,$$

так что

$$\langle \boldsymbol{k}_\mathrm{f} | V | \boldsymbol{k}_\mathrm{i} \rangle = \int \mathrm{d}^3 r V(\boldsymbol{r}) \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}_\mathrm{f} - \boldsymbol{k}_\mathrm{i})\cdot \boldsymbol{r}} = \tilde{V}\left(\boldsymbol{k}_\mathrm{f} - \boldsymbol{k}_\mathrm{i}\right),$$

где $\tilde{V}$ есть не что иное, как фурье-образ потенциала, зависящий от переданного импульса $\boldsymbol{q} = \hbar\left(\boldsymbol{k}_\mathrm{f} - \boldsymbol{k}_\mathrm{i}\right)$. В итоге амплитуда рассеяния

$$f(\theta) \approx -\frac{m}{2\pi\hbar^2}\tilde{V}\left(\boldsymbol{k}_\mathrm{f} - \boldsymbol{k}_\mathrm{i}\right).$$

Это приближение называется борновским.

Критерий применимости борновского приближения

Критерий применимости борновского приближения включает в себя два аспекта. Поскольку итерации в исследуемых интегральных уравнениях представляют собой разложение решения в ряд по теории возмущений, где в качестве такого возмущения выступает потенциал, степень сходимости ряда можно оценить, во-первых, по малости самой борновской поправки к волновой функции свободной частицы, а во-вторых, по относительной величине поправок высших порядков по возмущению к волновой функции или к сечению рассеяния. На практике обычно ограничиваются первым условием:

$$\left|\psi_\mathrm{i}^{(+)}(\boldsymbol{x}) - \psi_\mathrm{i}^{(0)}(\boldsymbol{x})\right| \ll \left|\psi_\mathrm{i}^{(0)}(\boldsymbol{x})\right|,$$

а значит, согласно $\left|\psi_\mathrm{i}^{(+)}(\boldsymbol{x}) - \psi_\mathrm{i}^{(0)}(\boldsymbol{x})\right| = \left|\int \mathcal{G}_E^{(0)}\left(\boldsymbol{x} - \boldsymbol{x}_1\right) V\left(\boldsymbol{x}_1\right) \psi_\mathrm{i}^{(+)}\left(\boldsymbol{x}_1\right) \mathrm{d}^3 x_1\right|$,

$$\left|\psi_\mathrm{i}^{(+)}(\boldsymbol{x}) - \psi_\mathrm{i}^{(0)}(\boldsymbol{x})\right| \approx \left|\int \mathcal{G}_E^{(0)}\left(\boldsymbol{x} - \boldsymbol{x}_1\right) V\left(\boldsymbol{x}_1\right) \psi_\mathrm{i}^{(0)}\left(\boldsymbol{x}_1\right) \mathrm{d}^3 x_1\right| \ll 1.$$

В качестве грубой оценки интеграла сверху можно взять интеграл от модулей сомножителей:

$$\left|\int \mathcal{G}_E^{(0)}\left(\boldsymbol{x} - \boldsymbol{x}_1\right) V\left(\boldsymbol{x}_1\right) \psi_\mathrm{i}^{(0)}\left(\boldsymbol{x}_1\right) \mathrm{d}^3 x_1\right| \leqslant \int \left|\mathcal{G}_E^{(0)}\left(\boldsymbol{x} - \boldsymbol{x}_1\right)\right| \left|V\left(\boldsymbol{x}_1\right)\right| \left|\psi_\mathrm{i}^{(0)}\left(\boldsymbol{x}_1\right)\right| \mathrm{d}^3 x_1$$

Тогда для потенциала, отличного от нуля в ограниченной области $r < a$, с характерным масштабом энергии $|V(r)| \sim V_0$, из

$$\left|\mathcal{G}_E^{(0)}\left(\boldsymbol{x} - \boldsymbol{x}_1\right)\right| \approx \frac{m}{2\pi\hbar^2}\frac{1}{a}, \quad \left|\psi_\mathrm{i}^{(0)}\left(x_1\right)\right| = 1$$

находим

$$\frac{mV_0}{\hbar^2}a^2 \ll 1.$$

Если ввести обозначение λ_0 для характерной длины волны частицы с энергией V_0:

$$V_0 = \frac{\hbar^2}{m\lambda_0^2}$$

Удобно обозначить характерную длину волны частицы с энергией V_0 как λ_0, тогда:

$$V_0 = \frac{\hbar^2}{m\lambda_0^2},$$

то условие применимости борновского приближения принимает вид

$$\frac{a^2}{\lambda_0^2} \ll 1.$$

Это означает, например, что в случае притягивающего потенциала частица с длиной волны λ_0 не помещается в яме размером a, т. е. в яме нет связанных состояний. В этом же приближении амплитуда рассеяния

$$f \sim \frac{m}{2\pi\hbar^2} V_0 \frac{4\pi}{3} a^3 \approx a \frac{a^2}{\lambda_0^2},$$

и полное сечение

$$\sigma \sim 4\pi |f|^2 \approx 4\pi a^2 \frac{a^4}{\lambda_0^4}.$$

Величину

$$\sigma_{\text{geom}} = 4\pi a^2$$

обычно называют геометрическим сечением. Поэтому условие применимости борновского приближения еще записывают в виде

$$\sigma \ll \sigma_{\text{geom}} ,$$

т. е. рассчитанное в борновском приближении полное сечение должно быть существенно меньше геометрического сечения.

Полученные ограничения на применимость приближения Борна можно ослабить, если рассмотреть различные кинематические условия рассеяния.

Медленные частицы ($kr \sim ka \ll 1$) в борновском приближении

В этом случае экспоненциальные множители в функции Грина и в падающей волне можно заменить единицами

$$\mathrm{e}^{\mathrm{i}kr} \approx \mathrm{e}^{\mathrm{i}ka} \approx 1.$$

Но это, по сути, повторяет общие рассуждения, приведенные выше, где был взят модуль этих экспоненциальных факторов, также равный единице, так что ограничение на величину потенциала остается прежним.

(пропишу это потом!)

Быстрые частицы ($kr \sim ka \gg 1$) в борновском приближении

Функция Грина при $|\boldsymbol{r} - \boldsymbol{r}'| \approx a$

$$\mathcal{G}_E^{(0)}(\boldsymbol{r} - \boldsymbol{r}') \sim \frac{m}{2\pi\hbar^2} \frac{1}{a} \mathrm{e}^{\mathrm{i}ka},$$

а волна де Бройля

$$\psi_i^{(0)}(\boldsymbol{r}') = \mathrm{e}^{\mathrm{i}kr' \cos\theta'} \sim \mathrm{e}^{\mathrm{i}ka\cos\theta'}$$

быстро осциллирует как функция от $r' \sim a$ и зануляет интеграл везде, кроме узкой области по углам:

$$\mathrm{e}^{\mathrm{i}ka\cos\theta'} \sim 1, \quad |\cos\theta'| \lesssim \frac{1}{ka} \ll 1.$$

Ограничивая область интегрирования по телесному углу этим конусом, легко находим критерий применимости борновского приближения для быстрых частиц

$$\frac{mV_0}{\hbar^2} a^2 \frac{1}{ka} \ll 1 \Leftrightarrow \frac{a^2}{\lambda_0^2} \ll ka,$$

что, конечно, значительно слабее условия для медленных частиц.

Пример применений

Как догадаться про это?

7.2.5 Lippmann–Schwinger Integral Scattering Theory (??)

(потренирую, потом пропишу её, мб больше раздел сделаю, пока есть что есть. в 1ю часть тоже добавлю!)

Суть и основные формулы

В отличие от выражения в виде «T-экспоненты» для оператора эволюции, в случае потенциала, зависящего от времени, метод функций Грина приводит к обычным интегральным выражениям. Однако здесь тоже есть сложности с упорядочиванием по времени при расчетах петлевых квантовых поправок: возникающие интегралы могут содержать расходимости, методам устранения которых посвящена теория перенормировок, выходящая за рамки данного курса.

Обзор уравнения Липпмана-Швингера

(тут его обсудим)

$$\psi_{\mathrm{i}}^{(+)}(\boldsymbol{x}) = \psi_{\mathrm{i}}^{(0)}(\boldsymbol{x}) + \int \mathcal{G}_E^{(0)}\left(\boldsymbol{x}-\boldsymbol{x}_1\right) V\left(\boldsymbol{x}_1\right) \psi_{\mathrm{i}}^{(+)}\left(\boldsymbol{x}_1\right) \mathrm{d}^3 x_1$$

Теория

Установим тождество для функции Грина, используя

$$\mathbb{1} = G_E^{(0)}\left(E - H^{(0)}\right) = G_E^{(0)}(E - \hat{H} + V).$$

Преобразуем её как:

$$\begin{aligned} G_E =& \mathbb{1} \cdot G_E = \\ =& G_E^{(0)}(E - \hat{H} + V) G_E = \\ =& G_E^{(0)}\left(\mathbb{1} + V G_E\right) = \\ =& G_E^{(0)} + G_E^{(0)} V G_E. \end{aligned}$$

В координатном представлении оно является интегральным:

$$\mathcal{G}_E\left(\boldsymbol{r}, \boldsymbol{r}'\right) = \mathcal{G}_E^{(0)}\left(\boldsymbol{r}-\boldsymbol{r}'\right) + \int \mathcal{G}_E^{(0)}\left(\boldsymbol{r}-\boldsymbol{r}_1\right) V\left(\boldsymbol{r}_1\right) \mathcal{G}_E\left(\boldsymbol{r}_1, \boldsymbol{r}'\right) \mathrm{d}^3 r_1$$

Это уравнение можно решать методом итераций, т. е. находить решение с любой точностью по степени потенциала. Такой подход эффективен, если ряд последовательных приближений быстро сходится, и этот метод лежит в основе теории возмущений.

Аналогично и для запаздывающей функции Грина, если ввести состояния $|x\rangle$, нормированные согласно

$$\langle x | x' \rangle = \delta^{(4)}\left(x - x'\right).$$

(?? к чему это??)

Тогда получим уравнение

$$G = G^{(0)} + G^{(0)} V G$$

или в интегральном виде

$$\mathcal{G}\left(x,x'\right)=\mathcal{G}^{(0)}\left(x-x'\right)+\int\mathcal{G}^{(0)}\left(x-x_1\right)V\left(x_1\right)\mathcal{G}\left(x_1,x'\right)\mathrm{d}^4x_1$$

Запаздывающая функция Грина переводит начальное состояние $\psi_{\mathrm{i}}^{(0)}(x')$ в состояние в момент времени $t>t'$, $\psi_{\mathrm{i}}^{(+)}(x)$ так что

$$\psi_{\mathrm{i}}^{(0)}(x)=\mathrm{i}\hbar\int\mathcal{G}^{(0)}\left(x-x'\right)\psi_{\mathrm{i}}^{(0)}\left(x'\right)\mathrm{d}^3x'$$

а также

$$\psi_{\mathrm{i}}^{(+)}(x)=\mathrm{i}\hbar\int\mathcal{G}\left(x,x'\right)\psi_{\mathrm{i}}^{(0)}\left(x'\right)\mathrm{d}^3x',$$

(??? выпишу выше эти формулы, с ними должно быть уже знакомство. не уверен в обозначениях Киселева, мб изменю их.)

Подставим $\mathcal{G}\left(x,x'\right)$, получим:

$$\psi_{\mathrm{i}}^{(+)}(x)=\psi_{\mathrm{i}}^{(0)}(x)+\int\mathcal{G}^{(0)}\left(x-x_1\right)V\left(x_1\right)\psi_{\mathrm{i}}^{(+)}\left(x_1\right)\mathrm{d}^4x_1.$$

(?? дальше можно подумать. мб начну параграф про стац случай)

В стационарном случае потенциал не зависит от времени $V(x)=V(\boldsymbol{x})$, и начальное асимптотическое состояние с энергией E_{i} дает стационарное решение уравнения Шрёдингера с той же энергией:

$$\psi_{\mathrm{i}}^{(+)}(x)=\mathrm{e}^{-\frac{i}{\hbar}E_{\mathrm{i}}t}\psi_{\mathrm{i}}^{(+)}(\boldsymbol{x}).$$

Поэтому, добавив также под интеграл экспоненту и обратную, интегральное уравнение сводится к виду

$$\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_{\mathrm{i}}t}\psi_{\mathrm{i}}^{(+)}(\boldsymbol{x})=\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_{\mathrm{i}}t}\psi_{\mathrm{i}}^{(0)}(\boldsymbol{x})+\int\frac{\mathrm{d}E\ \mathrm{d}t_1}{2\pi\hbar}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(E_{\mathrm{i}}-E)t_1}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}\int\mathcal{G}_E^{(0)}\left(\boldsymbol{x}-\boldsymbol{x}_1\right)V\left(\boldsymbol{x}_1\right)\psi_{\mathrm{i}}^{(+)}\left(\boldsymbol{x}_1\right)\mathrm{d}^3x_1$$

(??? и откуда там интегрирование по энергии??? максимально плохо написано у Киселева.)

или после сокращения временных факторов, запишем так называемое уравнение Липпмана-Швингера

$$\psi_{\mathrm{i}}^{(+)}(\boldsymbol{x})=\psi_{\mathrm{i}}^{(0)}(\boldsymbol{x})+\int\mathcal{G}_E^{(0)}\left(\boldsymbol{x}-\boldsymbol{x}_1\right)V\left(\boldsymbol{x}_1\right)\psi_{\mathrm{i}}^{(+)}\left(\boldsymbol{x}_1\right)\mathrm{d}^3x_1$$

Это интегральное уравнение для стационарной волновой функции в задаче рассеяния.

Физический смысл этого уравнения становится ясным, если записать стационарное уравнение Шрёдингера для $\psi_{\mathrm{i}}^{(+)}(\boldsymbol{x})$:

$$\left(E-H^{(0)}\right)\psi_{\mathrm{i}}^{(+)}(\boldsymbol{x})=V(\boldsymbol{x})\psi_{\mathrm{i}}^{(+)}(\boldsymbol{x}),$$

которое, естественно, следует из интегрального уравнения. Поэтому правую часть можно рассматривать в качестве источника в уравнении Шрёдингера

$$\left(E-H^{(0)}\right)\psi(\boldsymbol{x})=j(\boldsymbol{x}),$$

общее решение которого представляется в виде суммы решения для однородного уравнения без источников, т. е. $\psi_{\mathrm{i}}^{(0)}(\boldsymbol{x})$, и частного решения

$$\int\mathcal{G}_E^{(0)}\left(\boldsymbol{x}-\boldsymbol{x}_1\right)j\left(\boldsymbol{x}_1\right)\mathrm{d}^3x_1$$

Тогда подстановка в это соотношение источника $j(\boldsymbol{x})=V(\boldsymbol{x})\psi_{\mathrm{i}}^{(+)}(\boldsymbol{x})$ приводит к интегральному уравнению для стационарной волновой функции.

(очень плохо написано, на примерах или в другом месте разберу потом.)

О том, почему мы делаем именно так (??)

(оставшийся вопрос, зачем вообще такое мы рассматриваем?? с опытом придет понимание.)

Асимптотическое поведение на больших расстояниях и формула для сечения

Интегральное уравнение Липпмана-Швингера

$$\psi_{\mathrm{i}}^{(+)}(\boldsymbol{r}) = \psi_{\mathrm{i}}^{(0)}(\boldsymbol{r}) + \int \mathcal{G}_E^{(0)}\left(\boldsymbol{r}-\boldsymbol{r}'\right) V\left(\boldsymbol{r}'\right) \psi_{\mathrm{i}}^{(+)}\left(\boldsymbol{r}'\right) \mathrm{d}^3 r'$$

позволяет установить асимптотическое поведение волновой функции в задаче рассеяния при $r \to \infty$.

Исследуем интегральный член, оставляя вклад падающей волны $\psi_{\mathrm{i}}^{(0)}(\boldsymbol{r})$.

При $r \to \infty$ и ограниченном $r' < a$ функция Грина свободной частицы есть

$$\mathcal{G}_E^{(0)}\left(\boldsymbol{r}, \boldsymbol{r}'\right) = -\frac{m}{2\pi\hbar^2} \frac{\mathrm{e}^{\mathrm{i}k_E|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|} \simeq -\frac{m}{2\pi\hbar^2} \frac{\mathrm{e}^{\mathrm{i}k_E(r-\boldsymbol{n}\cdot\boldsymbol{r}')}}{r}, \quad \boldsymbol{n} = \frac{\boldsymbol{r}}{r}.$$

Подставив, имеем:

$$\psi_{\mathrm{i}}^{(+)}(\boldsymbol{r}) \simeq \psi_{\mathrm{i}}^{(0)}(\boldsymbol{r}) + \frac{\mathrm{e}^{\mathrm{i}k_{\mathrm{i}}r}}{r} f(\theta), \quad r \to \infty$$

где

$$f(\theta) = -\frac{m}{2\pi\hbar^2} \int \mathrm{d}^3 r' \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_E\cdot\boldsymbol{r}'} V\left(r'\right) \psi_{\mathrm{i}}^{(+)}\left(\boldsymbol{r}'\right)$$

Учтено, что оно работает при потенциалах, для которых этот интеграл сходится.

Здесь в силу сохранения энергии $k_E = k_{\mathrm{i}}$, и $\boldsymbol{k}_E = \boldsymbol{n}k_E$. Поскольку скалярная величина f зависит от двух векторов $\boldsymbol{k}_{\mathrm{i}}$ и $\boldsymbol{k}_E$ в случае центрально симметричного поля, она может определяться только скалярными величинами: квадратами векторов и их скалярным произведением $\boldsymbol{k}_{\mathrm{i}} \cdot \boldsymbol{k}_E = k_{\mathrm{i}}^2 \cos\theta$, а значит, f является функцией угла между этими векторами, как мы и записали выше.

Если фиксировать нормировку падающей волны, то

$$\psi_{\mathrm{i}}^{(+)}(\boldsymbol{r}) \simeq \mathrm{e}^{\mathrm{i}\boldsymbol{k}_{\mathrm{i}}\cdot\boldsymbol{r}} + \frac{\mathrm{e}^{\mathrm{i}k_{\mathrm{i}}r}}{r} f(\theta), \quad r \to \infty$$

(?? про нормировку пока не доехал)

Величину $f(\theta)$ называют амплитудой рассеяния.

Поток вероятности после рассеяния и сечение

Поток начальной волны $\psi_i^{(0)}(\boldsymbol{r})$

$$\boldsymbol{j}_{\mathrm{i}} = \frac{\hbar}{m}\boldsymbol{k}_{\mathrm{i}}$$

Для расчета потока вероятности

$$j = -\frac{\mathrm{i}\hbar}{2m}\left\{\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\right\}$$

вычислим в асимптотической области $r \to \infty$ градиент вклада рассеяния.

В полярных координатах в $\boldsymbol{\nabla} = \boldsymbol{e}_r \frac{\partial}{\partial r} + \boldsymbol{e}_\theta \frac{\partial}{r\partial\theta} + \boldsymbol{e}_\phi \frac{\partial}{r\sin\theta\partial\phi}$ при $r \to \infty$ угловые компоненты убывают как $\mathcal{O}\left(1/r^2\right)$, так что вклад дает только компонента вдоль радиус-вектора $\boldsymbol{e}_r = \boldsymbol{n}$:

$$\boldsymbol{\nabla}\frac{\mathrm{e}^{\mathrm{i}k_{\mathrm{i}}r}}{r} f(\theta) \approx \mathrm{i}k_{\mathrm{i}} \frac{\mathrm{e}^{\mathrm{i}k_{\mathrm{i}}r}}{r} f(\theta)\boldsymbol{n} = \mathrm{i}\boldsymbol{k}_E \frac{\mathrm{e}^{\mathrm{i}k_{\mathrm{i}}r}}{r} f(\theta).$$

Подставив, получаем поток вероятности рассеяния

$$\boldsymbol{j}_{\text{out}} = \frac{\hbar}{m}\boldsymbol{k}_E \frac{1}{r^2}|f(\theta)|^2.$$

Он зависит от угла рассеяния θ и является симметричным по полярному углу ϕ (в случае сферически симметричного потенциала).

В асимптотической области в малом телесном угле этот поток можно аппроксимировать плоской волной с волновым вектором $\boldsymbol{k}_\text{f} = \boldsymbol{n}k_\text{i}$ и нормировкой, которая определяет вероятность рассеяния. В самом деле, за счет потока вероятности через площадь на сфере радиуса r в телесном угле $\mathrm{d}\Omega$

$$\mathrm{d}\boldsymbol{s} = \boldsymbol{n} \cdot r^2 \, \mathrm{d}\Omega$$

вероятность рассеяния в единицу времени составляет

$$\mathrm{d}w = \boldsymbol{j}_{\text{out}} \cdot \mathrm{d}s = \frac{\hbar}{m}k_\text{i}|f(\theta)|^2 \, \mathrm{d}\Omega.$$

Следовательно, дифференциальное сечение рассеяния как функция амплитуды есть:

$$\mathrm{d}\sigma = |f(\theta)|^2 \, \mathrm{d}\Omega.$$

(в 1ю добавлю эти формулы, вроде полезные!)

Обзор применений (?!!!!!)

(пока хз, где конкретно она нужна)

Как догадаться до уравнения Липпмана-Швингера (??)

(?? суть не понял, так что на это тоже не отвечу еще.)

7.2.6 Expansion of the S-Matrix and T-Matrix

(!! снова с обозначениями проблемы, нужно указать их четче, тут много самых разных волновых функций.)

Теория (??)

Выражение $\mathcal{S}_\text{fi} = \lim_{t\to+\infty}\left\langle \psi_\text{f}^{(0)}(t)|\psi_\text{i}^{(+)}(t)\right\rangle$ можно вычислить, подставив уравнение Липпмана-Швингера для $\left|\psi_\text{f}^{(0)}(t)\right\rangle$, получим:

$$\mathcal{S}_{fi} = \left\langle \psi_\text{f}^{(0)}|\psi_i^{(0)}\right\rangle + \int \psi_\text{f}^{*(0)}(x)\mathcal{G}^{(0)}\left(x-x_1\right)V\left(x_1\right)\psi_i^{(+)}\left(x_1\right)d^4x_1 d^3\boldsymbol{x}$$

Здесь

$$\left\langle \psi_\text{f}^{(0)}|\psi_\text{i}^{(0)}\right\rangle = e^{-\frac{\mathrm{i}}{\hbar}(E_\text{i}-E_\text{f})t}\left\langle \boldsymbol{k}_\text{f}|\boldsymbol{k}_\text{i}\right\rangle = (2\pi)^3\delta\left(\boldsymbol{k}_\text{f}-\boldsymbol{k}_\text{i}\right)$$

И при $t > t_1$

$$\mathrm{i}\hbar\int \psi_\text{f}^{*(0)}(x)\mathcal{G}^{(0)}\left(x-x_1\right)d^3\boldsymbol{x} = \int \left\langle \boldsymbol{k}_\text{f}|\boldsymbol{k}\right\rangle \frac{d^3\boldsymbol{k}}{(2\pi)^3}\left\langle \boldsymbol{k}|\boldsymbol{x}_1\right\rangle e^{\frac{\mathrm{i}}{\hbar}(E_\text{i}-E)t+\frac{\mathrm{i}}{\hbar}Et_1} = \psi_\text{f}^{*(0)}\left(x_1\right)$$

(??? окей, что выше - не так уж понимаю, нужно основы про волновую функцию прописать лучше.)

Это есть функциональное выражение тождества Для унитарного оператора эволюции

$$U\left(t,t'\right)U\left(t',t\right)=\mathbb{1}\quad\rightarrow\quad U\left(t,t'\right)=U^{\dagger}\left(t',t\right)$$

которое означает, что этот оператор описывает также и эволюцию назад по времени.

(??? пока это совсем не понимаю, какая связь??)

(ну там мысль в том, что пара произведений так вот переходит в финальное состояние)

Поэтому интегральный член в матричном элементе $\mathcal{S}_{\mathfrak{fi}}$ записывается в виде

$$\int\psi_{\mathrm{f}}^{*(0)}\left(x_1\right)V\left(x_1\right)\psi_{\mathrm{i}}^{(+)}\left(x_1\right)d^4x_1$$

Однако в стационарном случае потенциал пс зависит от времени, а волновая функция $\psi_i^{(+)}(x)$ является решением стационарного уравнения Шредингера с энергией начального асимптотического состояния E_{i}, так что интегрирование по t_1 легко выполняется

$$\int dt_1 e^{\frac{\mathrm{i}}{\hbar}\left(E_{\mathrm{f}}-E_{\mathrm{i}}\right)t}=2\pi\hbar\delta\left(E_{\mathrm{f}}-E_{\mathrm{i}}\right)$$

В итоге, матричный элемент

$$\mathcal{S}_{\mathfrak{f}i}=(2\pi)^3\delta\left(\boldsymbol{k}_{\mathfrak{f}}-\boldsymbol{k}_{\mathfrak{i}}\right)-\mathrm{i}2\pi\delta\left(E_{\mathfrak{f}}-E_{\mathfrak{i}}\right)\int\psi_{\mathfrak{f}}^{*(0)}(\boldsymbol{r})V(r)\psi_{\mathfrak{i}}^{(+)}(\boldsymbol{r})d^3\boldsymbol{r}$$

В этом выражении первый член отвечает вкладу за счет падающей на мишень волны в задаче рассеяния

$$(2\pi)^3\delta\left(\boldsymbol{k}_{\mathfrak{f}}-\boldsymbol{k}_{\mathfrak{i}}\right)=\langle\boldsymbol{k}_{\mathfrak{f}}|\boldsymbol{k}_{\mathfrak{i}}\rangle$$

а второй можно записать через амплитуду рассеяния $f(\theta)$ согласно ее определению:

$$\int\psi_{\mathrm{f}}^{*(0)}(\boldsymbol{r})V(r)\psi_{\mathrm{i}}^{(+)}(\boldsymbol{r})d^3\boldsymbol{r}=\int d^3\boldsymbol{r}e^{-\mathrm{i}\boldsymbol{k}_{\mathrm{f}}\cdot\boldsymbol{r}}V(r)\psi_{\mathrm{i}}^{(+)}(\boldsymbol{r})=-\frac{2\pi\hbar^2}{m}f(\theta)$$

Важно подчеркнуть, что интегральное представление для волновой функции и матричного элемента позволило нам доказать сделанное при постановке задачи рассеяния утверждение, что амплитуда перехода пропорциональна дельта-функции от разности энергий начального и конечного асимптотического состояний, так что ее квадрат определяет вероятность перехода в единицу времени.

T-матрица

Поскольку S-матрица есть предельное значение оператора эволюции при бесконечном Времени эволюции, она, как частный случай оператора эволюции, унитарного в любой момент времени, также является унитарной

$$\mathcal{S}\mathcal{S}^{\dagger}=\mathbb{1}$$

Обычно вводят понятие T-матрицы рассеяния, чтобы исключить тривиальный вклад падающих на мишень волн из $\mathcal{S}$-матрицы

$$\mathcal{S}=1-\frac{i}{\hbar}\mathcal{T}.$$

Унитарность $\mathcal{S}$-матрицы дает

$$\left(\mathbb{1} - \frac{\mathrm{i}}{\hbar}\mathcal{T}\right)\left(\mathbb{1} + \frac{\mathrm{i}}{\hbar}\mathcal{T}^\dagger\right) = \mathbb{1},$$

откуда следует соотношение унитарности для $\mathcal{T}$ - матрицы

$$\mathcal{T}\mathcal{T}^\dagger = -2\hbar\,\mathrm{Im}\,\mathcal{T}$$

В стационарном случае

$$\mathrm{S_{fi}} = \langle \boldsymbol{k}_\mathrm{f}|\boldsymbol{k}_\mathrm{i}\rangle - \frac{\mathrm{i}}{\hbar}\langle \boldsymbol{k}_\mathrm{f}|\mathcal{T}|\boldsymbol{k}_\mathrm{i}\rangle = \langle \boldsymbol{k}_\mathrm{f}|\boldsymbol{k}_\mathrm{i}\rangle - \frac{\mathrm{i}}{\hbar}2\pi\hbar\delta\left(E_\mathrm{f} - E_\mathrm{i}\right)\left\langle \boldsymbol{k}_\mathrm{f}|V|\psi_\mathrm{i}^{(+)}\right\rangle,$$

то есть

$$\mathcal{T}_\mathrm{fi} = \langle \boldsymbol{k}_\mathrm{f}|\mathcal{T}|\boldsymbol{k}_\mathrm{i}\rangle = -2\pi\hbar\delta\left(E_\mathrm{f} - E_\mathrm{i}\right)\frac{2\pi\hbar^2}{m}f(\theta).$$

(?? пропишу там потом еще раз эти формулы, потому что не усвоено, что именно такие свойства S матрицы.)

Если взять диагональный матричный элемент соотношения унитарности для $\mathcal{T}$-матрицы

$$\left\langle \boldsymbol{k}_\mathrm{i}\left|\mathcal{T}\mathcal{T}^\dagger\right|\boldsymbol{k}_\mathrm{i}\right\rangle = -2\hbar\,\mathrm{Im}\,\langle \boldsymbol{k}_\mathrm{i}|\mathcal{T}|\boldsymbol{k}_\mathrm{i}\rangle,$$

то в правой части будет стоять величина

$$-2\hbar\,\mathrm{Im}\,\langle \boldsymbol{k}_\mathrm{i}|\mathcal{T}|\boldsymbol{k}_\mathrm{i}\rangle = 2\pi\hbar\delta(E)|_{E\to 0}\,\frac{4\pi\hbar^3}{m}\,\mathrm{Im}\,f(0),$$

где $f(0)$ - амплитуда упругого рассеяния вперед, и, как обычно, формально $2\pi\hbar\delta(E)|_{E\to 0} = T \to \infty$ - время наблюдения за частицей при рассеянии.

Для левой части тождества унитарности T-матрицы запишем

$$\left\langle \boldsymbol{k}_\mathrm{i}\left|\mathcal{T}\mathcal{J}^\dagger\right|\boldsymbol{k}_\mathrm{i}\right\rangle = \int \langle \boldsymbol{k}_\mathrm{i}|\mathcal{T}|\boldsymbol{k}_\mathrm{f}\rangle\,\frac{\mathrm{d}^3k_\mathrm{f}}{(2\pi)^3}\left\langle \boldsymbol{k}_\mathrm{f}\left|\mathcal{T}^\dagger\right|\boldsymbol{k}_\mathrm{i}\right\rangle = \int \frac{\mathrm{d}^3k_\mathrm{f}}{(2\pi)^3}\left|\mathcal{T}_\mathrm{fi}\right|^2.$$

Вероятность рассеяния в единицу времени через T-матрицу есть

$$\mathrm{d}w_\mathrm{fi} = \frac{\left|\mathcal{S}_\mathrm{fi}\right|^2}{T}\frac{\mathrm{d}^3k_\mathrm{f}}{(2\pi)^3} = \frac{\left|\mathcal{T}_\mathrm{fi}\right|^2}{\hbar^2 T}\frac{\mathrm{d}^3k_\mathrm{f}}{(2\pi)^3},$$

а полное сечение рассеяния

$$\sigma = \frac{1}{j_\mathrm{i}}\int \mathrm{d}w_\mathrm{fi} = \frac{1}{T\hbar^2 j_\mathrm{i}}\int \frac{\mathrm{d}^3k_\mathrm{f}}{(2\pi)^3}\left|\mathcal{T}_\mathrm{fi}\right|^2.$$

В итоге время наблюдения T в равенстве сокращается, и унитарность приводит к тождеству

$$\hbar^2 j_\mathrm{i}\sigma = \frac{4\pi\hbar^3}{m}\,\mathrm{Im}\,f(0),$$

так что с учетом $j_\mathrm{i} = \hbar k_\mathrm{i}/m$ окончательно находим

$$\sigma = \frac{4\pi}{k_\mathrm{i}}\,\mathrm{Im}\,f(0).$$

Это тождество составляет содержание оптической теоремы, или соотношения Бора-Пайерлса-Плачека, связывающего полное сечение рассеяния с мнимой частью амплитуды упругого рассеяния вперед.

(чуть улучшу верстку, также строчкой опишу идею вывода. вроде понял.)

Стационарная $\mathcal{T}_E$

Наконец, введем стационарную $\mathcal{T}$-матрицу

$$\mathcal{T} = 2\pi\hbar\delta\left(E_{\mathrm{f}} - E_{\mathrm{i}}\right)\mathcal{T}_E.$$

Тогда интегральное уравнение для состояния

$$\left|\psi_{\mathrm{i}}^{(+)}\right\rangle = \left|\psi_{\mathrm{i}}^{(0)}\right\rangle + G_E^{(0)} V \left|\psi_{\mathrm{i}}^{(+)}\right\rangle$$

позволяет установить для матричного элемента $\mathcal{T}_E$

$$\langle \boldsymbol{k_f} \left|\mathcal{T}_E\right| \boldsymbol{k}_{\mathrm{i}}\rangle = \left\langle \boldsymbol{k_f} | V | \psi_{\mathrm{i}}^{(+)} \right\rangle$$

следующее равенство

$$\begin{aligned}
\langle \boldsymbol{k}_{\mathrm{f}} \left|\mathcal{T}_E\right| \boldsymbol{k}_{\mathrm{i}}\rangle &= \langle \boldsymbol{k}_{\mathrm{f}} | V | \boldsymbol{k}_{\mathrm{i}}\rangle + \left\langle \boldsymbol{k}_{\mathrm{f}} \left| V G_E^{(0)} V \right| \psi_{\mathrm{i}}^{(+)} \right\rangle = \\
&= \langle \boldsymbol{k}_{\mathrm{f}} | V | \boldsymbol{k}_{\mathrm{i}}\rangle + \int \left\langle \boldsymbol{k}_{\mathrm{f}} \left| V G_E^{(0)} \right| \boldsymbol{k} \right\rangle \frac{\mathrm{d}^3 k}{(2\pi)^3} \left\langle \boldsymbol{k} | V | \psi_{\mathrm{i}}^{(+)} \right\rangle = \\
&= \langle \boldsymbol{k}_{\mathrm{f}} | V | \boldsymbol{k}_{\mathrm{i}}\rangle + \int \left\langle \boldsymbol{k}_{\mathrm{f}} \left| V G_E^{(0)} \right| \boldsymbol{k} \right\rangle \frac{\mathrm{d}^3 k}{(2\pi)^3} \langle \boldsymbol{k} \left|\mathcal{T}_E\right| \boldsymbol{k}_{\mathrm{i}}\rangle .
\end{aligned}$$

Или в операторной форме

$$\mathcal{T}_E = V + V G_E^{(0)} \mathcal{T}_E,$$

что позволяет строить итерационный ряд, сходящийся в теории возмущений по малому потенциалу.

Представление взаимодействия and S-matrix по Левитову Шитову

(??? про это еще остаются вопросы, так и не понял, почему это важно. потом подумаю.)

В теории возмущений гамильтониан записывают в виде $\widehat{\mathcal{H}} = \widehat{\mathcal{H}}_0 + \widehat{\mathcal{H}}_{\mathrm{int}}$, где $\widehat{\mathcal{H}}_0$ - невозмущенная часть, а $\widehat{\mathcal{H}}_{\mathrm{int}}$ -возмущенная.

Наиболее удобно работать в представлении взаимодействия, т. е. в представлении Гейзенберга невозмущенной задачи.

В качестве базиса этого представления используются зависящие от времени собственные состояния невозмущенного гамильтониана $\widehat{\mathcal{H}_0}$:

$$|\alpha\rangle(t) = e^{-(i/\hbar)E_\alpha t}|\alpha\rangle,$$

где E_α -спектр $\widehat{\mathcal{H}}_0$. Уравнение Шредингера, записанное в этом базисе, принимает вид

$$i\hbar\frac{\partial\tilde{\psi}}{\partial t} = \widehat{\mathcal{H}}_{\mathrm{int}}(t)\tilde{\psi}$$

где $\widehat{\mathcal{H}}_{\mathrm{int}}(t) = e^{(i/\hbar)\widehat{\mathcal{H}}_0 t}\widehat{\mathcal{H}}_{\mathrm{int}}\, e^{-(i/\hbar)\widehat{\mathcal{H}}_0 t}$, а обозначение $\tilde{\psi}$ указывает, что ψ берется в представлении взаимодействия.

Формальное решение записывается через S-матрицу, $\tilde{\psi}(t) = \widehat{S}(t)\tilde{\psi}(0)$, которая дается так называемой хронологической экспонентой:

$$\widehat{S}(t) = \mathrm{T}\exp\left[-\frac{i}{\hbar}\int\limits_0^t \widehat{\mathcal{H}}_{\mathrm{int}}(t')\,dt'\right] = \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int\limits_0^t\int\limits_0^{t_1}\ldots\int\limits_0^{t_{n-1}} \widehat{\mathcal{H}}_{\mathrm{int}}(t_1)\ldots\widehat{\mathcal{H}}_{\mathrm{int}}(t_n)\,dt_n\ldots dt_1$$

где $0 < t_n < ... < t_1 < t$. Преобразования $(2.1) - (2.3)$ имеют общий квантово механический характер: они применимы и к одночастичной и к многочастичной задачам.

В многочастичном случае, представляющем основной интерес, необходимо перейти к ψ -операторам, после чего члены ряд разложения S-матрицы становятся полиномами по операторам рождения и уничтожения.

Анализ операторной структуры этих выражений приводит к простым правилам вычисления средних (теорема Вика) и к диаграммной технике, дающей удобное графическое представление для разложения S -матрицы в ряд по взаимодействию.

Введем хронологическое произведение операторов, которое часто называют также T-упорядоченным произведением операторов, или просто T-произведением. Для бозе-операторов

$$\mathrm{T}\widehat{A}(x)\widehat{B}(x') = \begin{cases} \widehat{A}(x)\widehat{B}(x') & \text{если } t > t' \\ \widehat{B}(x')\,\hat{A}(x) & \text{если } t < t' \end{cases}$$

а для ферми-операторов

$$\mathrm{T}\widehat{A}(x)\widehat{B}(x') = \begin{cases} \widehat{A}(x)\hat{B}(x') & \text{при } t > t' \\ -\widehat{B}(x')\,\widehat{A}(x) & \text{при } t < t' \end{cases}$$

(??? и почему это так???)

Иначе говоря, при T-упорядочении операторов их переставляют так, чтобы моменты времени, в которые взяты операторы, возрастали справа налево. При этом знак перестановки соответствует их коммутационным соотношениям: « + » для бозонов, " - » для фермионов.

С помощью T-произведения операторов можно записать выражение для хронологической экспоненты в более привычном виде:

$$\widehat{S}(t) = \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar}\right)^n \frac{1}{n!} \mathrm{T}\left(\int_0^t \widehat{\mathcal{H}}_{\text{int}}(t')\,dt'\right)^n$$

7.2.7 Unitarity and the Optical Theorem

Теория оптической теоремы

она не применима в Борновском приближении. Тут об этом.

Optical theorem is applicable even if there are inelastic processes

The optical theorem follows from very basic conservation laws and as such has a very general nature. It is valid even for scattering of composite particles, where inelastic processes are possible. In the latter case, we should use in Eq. (XIII.11), the total collision cross-section for $\sigma(E)$, while $f(E, 0)$ should be understood as the forward-scattering amplitude of elastic scattering of the composite particle.

(???? why?? this is what Galitski wrote)

7.3 Scattering Theory: Phase Decomposition Approach

(I'll write formulas about it later)

8 Specific Methods and Templates

8.1 Path Integral Formulation of QM: Basics

8.1.1 1. Feynman Path Integral

Here we present Feynman's path integral approach to quantum mechanics, which expresses the propagator of a quantum system with the Hamiltonian H - the kernel of the evolution operator $U(t) = e^{-\frac{i}{\hbar}tH}$ - as a "sum over trajectories" of the corresponding classical system.

1.1. The fundamental solution of the Schrdinger equation.

Recall (see Section 1.3 of Chapter 2) that in terms of the evolution operator $U(t) = e^{-\frac{i}{\hbar}tH}$, the solution $\psi(t)$ of the initial value problem for the time-dependent Schrdinger equation

$$i\hbar\frac{d\psi}{dt}(t) = H\psi(t), \tag{1.1}$$

$$\psi(t)|_{t=0} = \psi \tag{1.2}$$

is given by $\psi(t) = U(t)\psi$. For the Hamiltonian operator

$$H = \frac{\boldsymbol{P}^2}{2m} + V(\boldsymbol{Q})$$

of a quantum particle in $\mathbb{R}^n$ moving in the potential field $V(\boldsymbol{q})$, the initial value problem (1.1)-(1.2) in coordinate representation becomes the following

Cauchy problem:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + V(\boldsymbol{q})\psi \tag{1.3}$$

$$\psi(\boldsymbol{q},t)|_{t=0} = \psi(\boldsymbol{q}) \tag{1.4}$$

where Δ is the Laplace operator on $\mathbb{R}^n$. Under rather general conditions on the potential $V(\boldsymbol{q})$ (i.e., when $V \in L^\infty_{\text{loc}}(\mathbb{R}^n)$ is bounded from below) the Cauchy problem (1.3)-(1.4) has a fundamental solution: a function $K(\boldsymbol{q},\boldsymbol{q}',t)$ which satisfies partial differential equation (1.3) with respect to the variable $\boldsymbol{q}$ in the distributional sense (i.e., $K(\boldsymbol{q},\boldsymbol{q}',t)$ is a weak solution of the Schrdinger equation), and the initial condition

$$K(\boldsymbol{q},\boldsymbol{q}',t)|_{t=0} = \delta(\boldsymbol{q}-\boldsymbol{q}') \tag{1.5}$$

The solution of the Cauchy problem (1.3)-(1.4) can be formally written as

$$\psi(\boldsymbol{q}',t) = \int_{\mathbb{R}^n} K(\boldsymbol{q}',\boldsymbol{q},t)\,\psi(\boldsymbol{q})d^n\boldsymbol{q} \tag{1.6}$$

where the integral is understood in the distributional sense.
For $\psi \in L^2(\mathbb{R}^n)$ formula (1.6) should be understood as

$$\psi(\boldsymbol{q}',t) = \operatorname*{li.m.}_{R\to\infty}\int_{|\boldsymbol{q}|\le R} K(\boldsymbol{q}',\boldsymbol{q},t)\,\psi(\boldsymbol{q})d^n\boldsymbol{q} = \text{l.i.m.}\int_{\mathbb{R}^n} K(\boldsymbol{q}',\boldsymbol{q},t)\,\psi(\boldsymbol{q})d^n\boldsymbol{q},$$

where l.i.m. stands for the limit in the L^2-norm. In general, $\psi(\boldsymbol{q},t)$ is only a weak solution of the Schrdinger equation (1.3), and it is a regular solution when ψ belongs to the Grding domain

D_0 (see Problem 1.7 in Section 1.3 of Chapter 2). The fundamental solution $K(\boldsymbol{q}, \boldsymbol{q}', t)$ is the distributional kernel (in the sense of the Schwartz kernel theorem) of the evolution operator $U(t)$.

Using the group property $U(t+t') = U(t)U(t')$, we can rewrite (1.6) in the form

$$\psi(\boldsymbol{q}', t') = \int_{\mathbb{R}^n} K(\boldsymbol{q}', t'; \boldsymbol{q}, t)\, \psi(\boldsymbol{q}, t) d^n\boldsymbol{q} \tag{1.7}$$

where $K(\boldsymbol{q}', t'; \boldsymbol{q}, t) = K(\boldsymbol{q}', \boldsymbol{q}, t'-t)$. The function $|K(\boldsymbol{q}', t'; \boldsymbol{q}, t)|^2$ has a physical meaning of conditional probability distribution of finding a quantum particle at a point $\boldsymbol{q}' \in \mathbb{R}^n$ at time t' provided that it was at the point $\boldsymbol{q} \in \mathbb{R}^n$ at time t.

Remark. In physics terminology, the distributional kernel $K(\boldsymbol{q}', t'; \boldsymbol{q}, t)$ of the evolution operator $U(t'-t)$ is called the complex probability amplitude, or simply the amplitude or propagator. In Dirac's notation, $K(\boldsymbol{q}', t'; \boldsymbol{q}, t) = \langle \boldsymbol{q}', t' | \boldsymbol{q}, t \rangle$.

Finding the propagator of a given quantum system is a fundamental problem of quantum mechanics. When the spectral decomposition of the Hamiltonian operator H is known, the propagator can be obtained in

a closed form. Namely, suppose for simplicity that H has a pure point spectrum, i.e., there is an orthonormal basis of the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^n, d^n\boldsymbol{q})$ consisting of the eigenfunctions $\{\psi_n(\boldsymbol{q})\}_{n=0}^{\infty}$ of H with the eigenvalues E_n. We have

$$\psi(\boldsymbol{q}) = \sum_{n=0}^{\infty} c_n \psi_n(\boldsymbol{q}), \quad c_n = \int_{\mathbb{R}^n} \psi(\boldsymbol{q}) \overline{\psi_n(\boldsymbol{q})} d^n\boldsymbol{q}$$

so that

$$(U(t)\psi)(\boldsymbol{q}) = \sum_{n=0}^{\infty} e^{-\frac{i}{\hbar}E_n t} c_n \psi_n(\boldsymbol{q})$$

and

$$\psi(\boldsymbol{q}', t') = \sum_{n=0}^{\infty} e^{-\frac{i}{\hbar}E_n t'} \psi_n(\boldsymbol{q}') \int_{\mathbb{R}^n} \overline{\psi_n(\boldsymbol{q})} \psi(\boldsymbol{q}) d^n\boldsymbol{q},$$

where the series and integrals converge in the L^2-sense. If the change of orders of summation and integration was justified, we could write

$$K(\boldsymbol{q}', t; \boldsymbol{q}, t) = \sum_{n=0}^{\infty} e^{-\frac{i}{\hbar}E_n T} \psi_n(\boldsymbol{q}') \overline{\psi_n(\boldsymbol{q})}, \quad T = t' - t \tag{1.8}$$

The series (1.8) converges in the distributional sense, and gives a representation of the propogator in terms of the spectral decomposition of H.

A similar representation of the propagator exists when the Hamiltonian H has absolutely continuous spectrum. Consider the simplest case of a free quantum particle with the Hamiltonian operator

$$H_0 = \frac{\boldsymbol{P}^2}{2m}.$$

The corresponding Schrdinger equation can be solved by the Fourier method (see Section 2.3 in Chapter 2), and we obtain

$$\psi(\boldsymbol{q}',t') = \text{ l.i.m. } (2\pi\hbar)^{-\frac{n}{2}} \int_{\mathbb{R}^n} e^{\frac{i}{\hbar}\left(\boldsymbol{q}'\boldsymbol{p}-\frac{p^2}{2m}T\right)} \hat{\psi}(\boldsymbol{p},t) d^n\boldsymbol{p}$$
$$= \text{ l.i.m. } \int_{\mathbb{R}^n} K(\boldsymbol{q}',t';\boldsymbol{q},t)\,\psi(\boldsymbol{q},t) d^n\boldsymbol{q}$$

where

$$K(\boldsymbol{q}',t';\boldsymbol{q},t) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} e^{\frac{i}{\hbar}\left(\boldsymbol{p}(\boldsymbol{q}'-\boldsymbol{q})-\frac{p^2}{2m}T\right)} d^n\boldsymbol{p}, \quad T = t'-t. \tag{1.9}$$

Using the classical Fresnel integral formula

$$\int_{-\infty}^{\infty} e^{iax^2} dx = e^{\frac{\pi i \operatorname{sgn}(a)}{4}} \sqrt{\frac{\pi}{|a|}} \tag{1.10}$$

and completing the square in (1.9), we obtain the following expression for the propagator of a free quantum particle:

$$K(\boldsymbol{q}',t';\boldsymbol{q},t) = \left(\frac{m}{2\pi i\hbar T}\right)^{\frac{n}{2}} e^{\frac{im}{2\hbar T}(\boldsymbol{q}-\boldsymbol{q}')^2} \tag{1.11}$$

where $i^{\frac{n}{2}} = e^{-\frac{\pi i n}{4}}$ and $T > 0$.

Remark. Formally replacing the actual "physical" time t in the Schrdinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi$$

for a free quantum particle of mass m by the Euclidean time (or pure imaginary time) $-it$, we obtain the heat (diffusion) equation

$$\frac{1}{D}\frac{\partial u}{\partial t} = \Delta u$$

on $\mathbb{R}^n$ with the diffusion coefficient $D = \frac{\hbar}{2m}$. It is quite remarkable that in agreement with this formal procedure the propagator (1.11) for a free quantum particle is obtained from the heat kernel on $\mathbb{R}^n$ by the analytic continuation $T \mapsto -iT$.

Problem 1.1. Show that

$$\lim_{R\to\infty}\int_0^R \sin x^2 dx = \lim_{R\to\infty}\int_0^R \cos x^2 dx = \frac{1}{2}\sqrt{\frac{\pi}{2}}$$

by integrating the function e^{-z^2} over an appropriate "pizza-sliced" contour.

Problem 1.2. Show directly that

$$\psi(\boldsymbol{q}',t) = \left(e^{-\frac{i}{\hbar}tH_0}\psi\right)(\boldsymbol{q}') = \text{ l.i.m. } \left(\frac{m}{2\pi i\hbar t}\right)^{\frac{n}{2}} \int_{\mathbb{R}^n} e^{\frac{im}{2\hbar t}(\boldsymbol{q}-\boldsymbol{q}')^2}\psi(\boldsymbol{q}) d^n\boldsymbol{q}.$$

Problem 1.3. Give an expression for the propagator when H is a Schrdinger operator with rapidly decreasing potential, considered in Section 2 in Chapter 3.

1.2. Feynman path integral in the phase space. For a general Hamiltonian operator $H = H_0 + V$, where $V = V(\boldsymbol{Q})$, there is no simple formula for the propagator $K(\boldsymbol{q}',t';\boldsymbol{q},t)$ like (1.11). This is because operators H_0 and V do not commute, so that $e^{-\frac{i}{\hbar}tH} \neq e^{-\frac{i}{\hbar}tH_0}e^{-\frac{i}{\hbar}tV}$.

It was Feynman's fundamental discovery that there is another representation of the propagator for a quantum system in terms of the corresponding classical system. We start by describing Feynman's approach for the case of a quantum particle with one degree of freedom. It is based on the so-called Lie-Kato-Trotter product formula, which allows us to express the exponential

$e^{i(A+B)}$ of two non-commuting self-adjoint operators in terms of the individual exponentials e^{iA} and e^{iB}.

Theorem 1.1 (Lie-Kato-Trotter product formula). Let A and B be selfadjoint operators on $\mathscr{H}$ such that $A+B$ is essentially self-adjoint on $D(A)\cap D(B)$. Then for $\psi\in\mathscr{H}$,

$$e^{i(A+B)}\psi=\lim_{n\to\infty}\left(e^{\frac{i}{n}A}e^{\frac{i}{n}B}\right)^n\psi$$

Proof. We consider only the special case when A and B are bounded operators, which was already proved by Sophus Lie. Set $C_n=e^{i(A+B)/n}$ and $D_n=e^{iA/n}e^{iB/n}$. We have the telescopic sum

$$\begin{aligned}C_n^n-D_n^n&=C_n^n-C_n^{n-1}D_n+C_n^{n-1}D_n-C_n^{n-2}D_n^2+\cdots+C_nD_n^{n-1}-D_n^n\\&=\sum_{k=0}^{n-1}C_n^{n-k-1}\left(C_n-D_n\right)D_n^k\end{aligned}$$

and since by the Taylor formula $\|C_n-D_n\|\leq\frac{c}{n^2}$ for some constant $c>0$, we obtain

$$\|C_n^n-D_n^n\|\leq\frac{c}{n}$$

This proves the result with convergence in the uniform topology.
We will always assume that the Hamiltonian $H=H_0+V$ is essentially self-adjoint on $D\left(H_0\right)\cap D(V)$, so that the Lie-Kato-Trotter formula is applicable. (According to Theorem 1.2 in Section 1.1 of Chapter 3, for the case $n=3$ we can assume that $V=V_1+V_2$, where $V_1\in L^2\left(\mathbb{R}^3\right)$ and $V_2\in L^\infty\left(\mathbb{R}^3\right)$.) Applying the Lie-Kato-Trotter formula to $A=-\frac{T}{\hbar}H_0$ and $B=-\frac{T}{\hbar}V$, we obtain that in the strong operator topology

$$e^{-\frac{i}{\hbar}TH}=\lim_{n\to\infty}\left(e^{-\frac{i\Delta t}{\hbar}H_0}e^{-\frac{i\Delta t}{\hbar}V}\right)^n,\quad\Delta t=\frac{T}{n}\tag{1.12}$$

where $T=t'-t$. In the coordinate representation the operator $e^{-\frac{i\Delta t}{\hbar}V}$ is a multiplication by $e^{-\frac{i}{\hbar}V(q)\Delta t}$ operator, and the distributional kernel of the operator $e^{-\frac{i\Delta t}{\hbar}H_0}$ is given by (1.9), where T is replaced by Δt. Thus the distributional kernel $K\left(q',q;\Delta t\right)$ of the operator $e^{-\frac{i\Delta t}{\hbar}H_0}e^{-\frac{i\Delta t}{\hbar}V}$ is given by

$$K\left(q',q;\Delta t\right)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}e^{\frac{i}{\hbar}\left(p(q'-q)-\left(\frac{p^2}{2m}+V(q)\right)\Delta t\right)}dp\tag{1.13}$$

Since the kernel of a product of two operators is a composition of corresponding individual kernels, for the distributional kernel $K_n\left(q',t';q,t\right)$ of the operator $\left(e^{-\frac{i\Delta t}{\hbar}H_0}e^{-\frac{i\Delta t}{\hbar}V}\right)^n$ we obtain the following integral representation:

$$K_n\left(q',t';q,t\right)=\int\ldots\int\prod_{k=0}^{n-1}K\left(q_{k+1},q_k;\Delta t\right)\prod_{k=1}^{n-1}dq_k\tag{1.14}$$

where $q_0=q,q_n=q'$. Now replace each factor $K\left(q_{k+1},q_k;\Delta t\right)$ in (1.14) by its integral representation (1.13), where the corresponding variable of integration is denoted by $p_k,k=0,\ldots,n-1$. Changing the order of integrations in the resulting $(2n-1)$-fold integral and using (1.12), we obtain the following remarkable representation of the propagator of a quantum particle as a limit of multiple integrals when the number of integrations goes to infinity:

$$K\left(q',t';q,t\right)=\lim_{n\to\infty}K_n\left(q',t';q,t\right)\tag{1.15}$$

$= \lim_{n\to\infty} \int_{\mathbb{R}^{2n-1}} ... \int \exp\left\{ \frac{i}{\hbar} \sum_{k=0}^{n-1} \left(p_k \left(q_{k+1} - q_k \right) - H_c \left(p_k, q_k \right) \Delta t \right) \right\} \frac{dp_0}{2\pi\hbar} \prod_{k=1}^{n-1} \frac{dp_k dq_k}{2\pi\hbar}$.
Here $H_c(p,q) = \frac{p^2}{2m} + V(q)$ is the classical Hamiltonian function, and $q_0 = q, q_n = q'$.

Heuristically, formula (1.15) admits the following interpretation. To every point $(p_0, p_1, ..., p_{n-1}, q_1, ..., q_{n-1}) \in \mathbb{R}^{2n-1}$ assign a piece-wise linear path σ in the extended phase space $\mathbb{R}^2 \times \mathbb{R}$ of the classical particle, defined by the following time slicing procedure. Let $t_k = t + k\Delta t$ and $\sigma(\tau) = (p(\tau), q(\tau), \tau)$, where

$$p(\tau) = p_k, \quad q(\tau) = q_k + (\tau - t_k) \frac{q_{k+1} - q_k}{t_{k+1} - t_k}$$

and $\tau \in [t_k, t_{k+1}], k = 0, ..., n-1$. Then for the Riemann integrable potentials $V(q)$ we have

$$\sum_{k=0}^{n-1} \left(p_k \left(q_{k+1} - q_k \right) - H_c \left(p_k, q_k \right) \Delta t \right) = S(\sigma) + o(1), \quad \text{as} \quad n \to \infty \tag{1.16}$$

where

$$S(\sigma) = \int_\sigma \left(pdq - H_c d\tau \right) = \int_t^{t'} \left(p(\tau)\dot{q}(\tau) - H_c(p(\tau), q(\tau)) \right) d\tau$$

is the action functional of a classical system with the Hamiltonian function $H_c(p,q)$ (see Section 2.2 in Chapter 1). This suggests to interpret (1.15) as a kind of "integral" over the space $\tilde{P}\left(\mathbb{R}^2\right)_{q,t}^{q,t'}$ of all paths $\sigma(\tau) = (p(\tau), q(\tau), \tau)$ in the extended phase space $\mathbb{R}^2 \times \mathbb{R}$ such that ${}^1q(t) = q$ and $q\left(t'\right) = q'$, which was used in the formulation of the principle of the least action in the phase space (see Section 2.2 in Chapter 1). Thus we put

$$K\left(q', t'; q, t\right) = \int_{\tilde{P}(\mathbb{R}^2)_{q,t}^{q',t'}} e^{\frac{i}{\hbar} S(\sigma)} \mathscr{D}p\mathscr{D}q \tag{1.17}$$

where the "measure" $\mathscr{D}p\mathscr{D}q$ on $\tilde{P}\left(\mathbb{R}^2\right)_{q,t}^{q',t'}$ is given by

$$\mathscr{D}p\mathscr{D}q = \lim_{n\to\infty} \frac{dp_0}{2\pi\hbar} \prod_{k=1}^{n-1} \frac{dp_k dq_k}{2\pi\hbar}. \tag{1.18}$$

Representation (1.17)-(1.18) is the famous Feynman path integral in the phase space for the propagator of a quantum particle. It expresses the propagator $K\left(q', t'; q, t\right)$ as the "weighted sum" over all possible "histories" of the classical particle, the paths $\sigma \in \tilde{P}\left(\mathbb{R}^2\right)_{q,t}^{q',t'}$, where each path σ has a complex weight $\exp\left\{ \frac{i}{\hbar} S(\sigma) \right\}$. On one hand, this representation clearly shows the fundamental difference between classical mechanics and quantum mechanics. Thus in classical mechanics, the particle moves along classical trajectories, which are the critical points (extremals) of the action functional $S(\sigma)$, whereas in quantum mechanics all possible paths contribute to the complex probability amplitude $K\left(q', t'; q, t\right)$. On the other hand, representation (1.17)-(1.18) clearly points at the relation between quantum mechanics and classical mechanics in the semi-classical limit $\hbar \to 0$. Namely, as $\hbar \to 0$ the weights $\exp\left\{ \frac{i}{\hbar} S(\sigma) \right\}$ become rapidly oscillating and their contributions to (1.17) will mutually cancel, unless the action is almost constant. The latter happens near the critical points, which give the major contribution to (1.17). This is how classical trajectories of a particle emerge from its quantum description, which will be discussed in detail in Section 6.1.

Remark. The Feynman path integral in the phase space in not an integral in the sense of abstract integration theory, since the formal expression $\mathscr{D}p\mathscr{D}q$ does not define a measure [2] on

[01] Note that there is no condition on the values of $p(\tau)$ at the endpoints.

the path space $\tilde{P}\left(\mathbb{R}^2\right)_{q,t}^{q',t'}$. Besides, the functional $\exp\left\{\frac{i}{\hbar}S(\sigma)\right\}$ has absolute value 1 and cannot be integrable with respect to any measure $d\mu$ with the property $\mu\left(\tilde{P}\left(\mathbb{R}^2\right)_{q,t}^{q',t'}\right)=\infty$. The rigorous mathematical meaning of (1.17)-(1.18) is the original formula (1.15), which expresses the propagator as a limit of multiple integrals as the number of integrations goes to infinity. This explains the apparent "paradox" that quantum mechanics is defined entirely in classical terms by (1.17). It is not so, since there is no "intrinsic" definition of (1.17) in classical terms, besides the time slicing procedure (1.15), which also requires the special choice of the approximation (1.16) of $S(\sigma)$ by the Riemann sums.

1.3. Feynman path integral in the configuration space. Using the Fresnel integral (1.10) for the integration over p in (1.13), we obtain the following formula for the distributional kernel of the operator $e^{-\frac{i\Delta t}{\hbar}H_0}e^{-\frac{i\Delta t}{\hbar}V}$:

$$\sqrt{\frac{m}{2\pi i\hbar\Delta t}}e^{\frac{i}{\hbar}\left\{\frac{m}{2}\frac{(q-q')^2}{\Delta t}-V(q)\Delta t\right\}}$$

Repeating the time slicing procedure from the previous section, instead of (1.15) we now get

$$K\left(q',t';q,t\right)=\lim_{n\to\infty}\left(\frac{m}{2\pi\hbar i\Delta t}\right)^{\frac{n}{2}} \tag{1.19}$$
$$\times\int_{\mathbb{R}^{n-1}}...\int\exp\left\{\frac{i}{\hbar}\sum_{k=0}^{n-1}\left(\frac{m}{2}\left(\frac{q_{k+1}-q_k}{\Delta t}\right)^2-V\left(q_k\right)\right)\Delta t\right\}\prod_{k=1}^{n-1}dq_k$$

Assuming that $q_k=q\left(t_k\right),k=0,...,n$, for some smooth path $\gamma(\tau)=q(\tau)$ in $\mathbb{R}$, where $q_0=q$ and $q_n=q'$, we obtain as $n\to\infty$,

$$\sum_{k=0}^{n-1}\left(\frac{m}{2}\left(\frac{q_{k+1}-q_k}{\Delta t}\right)^2-V\left(q_k\right)\right)\Delta t=S(\gamma)+o(1)$$

where

$$S(\gamma)=\int_t^{t'}L\left(\gamma'(\tau)\right)d\tau=\int_t^{t'}L(q(\tau),\dot{q}(\tau))d\tau,\quad L(q,\dot{q})=\frac{1}{2}m\dot{q}^2-V(q)$$

is the action functional of a classical particle of mass m moving in the potential field $V(q)$ (see Section 1.3 in Chapter 1). This suggests to interpret the limit of multiple integrals (1.19) as the Feynman path integral in the configuration space

$$K\left(q',t';q,t\right)=\int_{P(\mathbb{R})_{q,t}^{q,tt'}}e^{\frac{i}{\hbar}S(\gamma)}\mathscr{D}q \tag{1.20}$$

Here $P(\mathbb{R})_{q,t}^{q',t'}$ is the space of smooth parametrized paths γ in the configuration space $\mathbb{R}$ connecting points q and q', and the "measure" $\mathscr{D}q$ on $P(\mathbb{R})_{q,t}^{q',t'}$ is given by

$$\mathscr{D}q=\lim_{n\to\infty}\left(\frac{m}{2\pi\hbar i\Delta t}\right)^{\frac{n}{2}}\prod_{k=1}^{n-1}dq_k \tag{1.21}$$

As the Feynman path integral in the phase space, the Feynman path integral in the configuration space is not actually an integral in the sense of integration theory, and the correct

[02] In abstract measure theory the measure is non-negative and countably additive.

mathematical meaning of (1.20)-(1.21) is given by (1.19). Formula (1.20) expresses the propagator $K(q',t';q,t)$ as the sum over all histories in the configuration space of classical particle - paths $\gamma \in P(\mathbb{R})_{q,t}^{q',t'}$, by assigning to each path γ a complex weight $\exp\left\{\frac{i}{\hbar}S(\gamma)\right\}$.

Remark. Convergence in (1.19), as well as in (1.15), is understood in the distributional sense. In particular, for every $\psi \in L^2(\mathbb{R})$,

$$\left(e^{-\frac{i}{\hbar}TH}\psi\right)(q) = \lim_{n\to\infty}\left(\frac{m}{2\pi\hbar i\Delta t}\right)^{\frac{n}{2}}$$
$$\times\int\cdots\int\exp\left\{\frac{i}{\hbar}\sum_{k=0}^{n-1}\left(\frac{m}{2}\left(\frac{q_{k+1}-q_k}{\Delta t}\right)^2 - V(q_k)\right)\Delta t\right\}\psi(q_n)\prod_{k=1}^{n}dq_k,$$

where all integrals are understood as $\int_{-\infty}^{\infty} = \lim_{R\to\infty}\int_{|q|\le R}$, and all limits — in the L^2-sense.

Remark. It is said in physics textbooks that the Feynman path integral in the configuration space is obtained from the Feynman path integral in the phase space by evaluating the Fresnel integral over $\mathscr{D}p$,

$$\int_{P(\mathbb{R})_{q,t}^{q',t'}} e^{\frac{i}{\hbar}\int_t^{t'}\left(\frac{m}{2}\dot{q}^2 - V(q)\right)d\tau}\mathscr{D}q = \int_{\tilde{P}(\mathbb{R}^2)_{q,t}^{q',t'}} e^{\frac{i}{\hbar}\int_t^{t'}(p\dot{q}-H_{\mathrm{c}}(p,q))d\tau}\mathscr{D}p\mathscr{D}q. \tag{1.22}$$

Note that the symbol $\mathscr{D}q$ has two different meanings: in the left-hand side of (1.22) it is defined by (1.21), whereas in the right-hand side it is defined as a part of (1.18).

1.4. Several degrees of freedom.

Let

$$H = \frac{\boldsymbol{P}^2}{2m} + V(\boldsymbol{Q})$$

be the Hamiltonian operator of a quantum particle in $\mathbb{R}^n$ moving in the potential field $V(\boldsymbol{q})$. As in the case of one degree of freedom, by using the Lie-Kato-Trotter product formula, the propagator $K(\boldsymbol{q}',t';\boldsymbol{q},t)$ is expressed as a limit of multiple integrals when the number of integrations goes to infinity,

$$K(\boldsymbol{q}',t';\boldsymbol{q},t) = \lim_{N\to\infty}\int_{\mathbb{R}^{(2N-1)n}}\cdots\int \tag{1.23}$$
$$\exp\left\{\frac{i}{\hbar}\sum_{k=0}^{N-1}\left(\boldsymbol{p}_k(\boldsymbol{q}_{k+1}-\boldsymbol{q}_k) - H_{\mathrm{c}}(\boldsymbol{p}_k,\boldsymbol{q}_k)\Delta t\right)\right\}\frac{d^n\boldsymbol{p}_0}{(2\pi\hbar)^n}\prod_{k=1}^{N-1}\frac{d^n\boldsymbol{p}_k d^n\boldsymbol{q}_k}{(2\pi\hbar)^n}.$$

Here $H_{\mathrm{c}}(\boldsymbol{p},\boldsymbol{q}) = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{q})$ is the classical Hamiltonian function, and $\boldsymbol{q}_0 = \boldsymbol{q}, \boldsymbol{q}_N = \boldsymbol{q}'$. This representation is symbolized by the Feynman path integral in the phase space $\mathscr{M} = T^*\mathbb{R}^n$,

$$K(\boldsymbol{q}',t';\boldsymbol{q},t) = \int_{\tilde{P}(\mathscr{M})_{\boldsymbol{q},t}^{\boldsymbol{q},t'}} e^{\frac{i}{\hbar}\int_\sigma(\boldsymbol{p}\dot{\boldsymbol{q}}-H_{\mathrm{c}}(\boldsymbol{p},\boldsymbol{q}))d\tau}\mathscr{D}\boldsymbol{p}\mathscr{D}\boldsymbol{q}, \tag{1.24}$$

where

$$\mathscr{D}\boldsymbol{p}\mathscr{D}\boldsymbol{q} = \lim_{N\to\infty}\frac{d^n\boldsymbol{p}_0}{(2\pi\hbar)^n}\prod_{k=1}^{N-1}\frac{d^n\boldsymbol{p}_k d^n\boldsymbol{q}_k}{(2\pi\hbar)^n}$$

and $\tilde{P}(\mathscr{M})_{q,t}^{\boldsymbol{q}',t'}$ is the space of all admissible paths σ in the extended phase space $\mathscr{M}\times\mathbb{R}$ connecting points $(\boldsymbol{q},t)$ and $(\boldsymbol{q}',t')$ (see Section 2.2 in Chapter 1).

Equivalently, the propagator $K(\boldsymbol{q}',t';\boldsymbol{q},t)$ can be written as

$$K(\boldsymbol{q}',t';\boldsymbol{q},t)=\lim_{N\to\infty}\left(\frac{m}{2\pi\hbar i\Delta t}\right)^{\frac{nN}{2}} \tag{1.25}$$
$$\times\int_{\mathbb{R}^{(n-1)}N}\cdots\int_{N}\exp\left\{\frac{i}{\hbar}\sum_{k=0}^{N-1}\left(\frac{m}{2}\left(\frac{\boldsymbol{q}_{k+1}-\boldsymbol{q}_k}{\Delta t}\right)^2-V(\boldsymbol{q}_k)\right)\Delta t\right\}\prod_{k=1}^{N-1}d^n\boldsymbol{q}_k$$

This formula is symbolized by the Feynman path integral in the configuration space,

$$K(\boldsymbol{q}',t';\boldsymbol{q},t)=\int_{P(M)_{q,t}^{q',t'}}e^{\frac{i}{\hbar}\int_t^{t'}L(\boldsymbol{q},\dot{\boldsymbol{q}})d\tau}\mathscr{D}\boldsymbol{q}, \tag{1.26}$$

where $L(\boldsymbol{q},\dot{\boldsymbol{q}})=\frac{1}{2}m\dot{\boldsymbol{q}}^2-V(\boldsymbol{q})$ is the corresponding Lagrangian,

$$\mathscr{D}\boldsymbol{q}=\lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{nN}{2}}\prod_{k=1}^{N-1}d^n\boldsymbol{q}_k,$$

and $P(M)_{\boldsymbol{q},t}^{\boldsymbol{q}'_t,t'}$ is the space of smooth parametrized paths in the configuration space M connecting points $\boldsymbol{q}$ and $\boldsymbol{q}'$. The precise mathematical meaning of formula (1.26) is the same as of (1.20).

Remark. Formally, definition (1.24) of the Feynman path integral in the phase space can be extended to the case $(\mathscr{M},\omega,H_c)$, where $\mathscr{M}=T^*M$ and $\omega=d\theta$, the canonical Liouville 1 -form on $\mathscr{M}$. Namely, one can obtain a distributional kernel $K(\boldsymbol{q}',t';\boldsymbol{q},t)$ by using the same time slicing as in (1.24) and replacing the 1 -form $\boldsymbol{p}d\boldsymbol{q}$ by θ, and the volume form $d^n\boldsymbol{p}_kd^n\boldsymbol{q}_k$ by an appropriate multiple of the Liouville volume form on $\mathscr{M}$. Similarly, representation (1.26) can be formally extended to the case of general Lagrangian system (M,L), where the configuration space M is a Riemannian manifold, by using the same time slicing and replacing $d^n\boldsymbol{q}_k$ by the Riemannian volume form on M. However, in general it is not clear for which unitary operators these Feynman integrals are actual distributional kernels. Moreover, even in the case $M=\mathbb{R}^n$ with the standard Euclidean metric, representations (1.26) and (1.24), where H_c is a Legendre transform of L, do not necessarily agree if L is not of the form "kinetic energy minus potential energy". However,
when $L=\frac{1}{2}g_{\mu\nu}(\boldsymbol{x})\dot{x}^\mu\dot{x}^\nu-V(\boldsymbol{x})$ (cf. Example 1.7 in Section 1.3 of Chapter 1), then with appropriately defined time slicing, Feynman path integrals (1.26) and (1.24) agree, and are equal to the propagator for the Hamiltonian operator

$$H=\frac{\hbar^2}{2}\Delta_g+V$$

Here Δ_g is the Laplace operator of the Riemannian metric on M, introduced in Example 2.4 in Section 2.4 of Chapter 2.

Remark. Formula (1.24) could serve as a heuristic tool which enables us, in some cases, to quantize the classical Hamiltonian system $(\mathscr{M},\omega,H_c)$. In general this is a rather non-trivial problem, especially when the phase space $\mathscr{M}$ is a compact manifold.

8.1.2 2. Symbols of the evolution operator and path integrals

In Sections 2.7 and 3.3 of Chapter 2 we introduced Wick, $\boldsymbol{pq-qqp}$-, and Weyl symbols of operators. For the evolution operator $U(T)=e^{-\frac{i}{\hbar}TH}$ these symbols can also be represented by Feynman path integrals. Here we consider only the case of one degree of freedom, since generalization to several degrees of freedom is straightforward.

2.1. The pq-symbol. Let $F_1(p,q,T)$ be the pq-symbol of the evolution operator $U(T)$. Using

(1.15) and formula (3.18) in Section 3.3 of Chapter 2 - the relation between the pq-symbol of an operator and its distributional kernel - we get

$$F_1(p,q,T)=\int_{-\infty}^{\infty}K(q-v,T;q,0)e^{\frac{i}{\hbar}pv}dv \tag{2.1}$$

$$=\lim_{n\to\infty}\int_{\mathbb{R}^{2n-2}}...\int\exp\left\{\frac{i}{\hbar}\sum_{k=0}^{n-1}\left(p_k\left(q_{k+1}-q_k\right)-H_{\mathrm{c}}\left(p_k,q_k\right)\Delta t\right)\right\}\prod_{k=1}^{n-1}\frac{dp_{k-1}dq_k}{2\pi\hbar}$$

where $p_{n-1}=p$ and $q_0=q_n=q$. Formula (2.1) can also be obtained from the composition formula for pq-symbols (see Problem 3.9 in Section 3.4 of Chapter 2). Indeed, it is sufficient to observe that the pq-symbol of the operator $e^{-\frac{i\Delta t}{\hbar}H_0}e^{-\frac{i\Delta t}{\hbar}V}$ is $f(p,q)=e^{-\frac{i\Delta t}{\hbar}H_c(p,q)}$, and to represent the pq-symbol of the operator $\left(e^{-\frac{i\Delta t}{\hbar}H_0}e^{-\frac{i\Delta t}{\hbar}V}\right)^n$ as the multiple integral

$$\int_{\mathbb{R}^{2n-2}}\cdots\int f\left(p,q_{n-1}\right)f\left(p_{n-2},q_{n-2}\right)\cdots f\left(p_2,q_2\right)f\left(p_0,q\right)$$
$$\times\exp\left\{\frac{i}{\hbar}\sum_{k=0}^{n-2}\left(p-p_k\right)\left(q_k-q_{k+1}\right)\right\}\prod_{k=1}^{n-1}\frac{dp_{k-1}dq_k}{2\pi\hbar}$$

where $q_0=q$. In the same spirit as (1.15), formula (2.1) can be written as the following Feynman path integral for the pq-symbol:

$$F_1(p,q,T)=\int_{\Omega_{(p,q)}(\mathbb{R}^2)}e^{\frac{i}{\hbar}S(\sigma)}\mathscr{D}p\mathscr{D}q,\quad S(\sigma)=\int_{\sigma}(pdq-H_{\mathrm{c}}dt) \tag{2.2}$$

where $\Omega_{(p,q)}\left(\mathbb{R}^2\right)=\left\{\sigma:[0,T]\to\mathbb{R}^2:\sigma(0)=\sigma(T)=(p,q)\in\mathbb{R}^2\right\}$ is the space of parametrized loops in the phase space $\mathbb{R}^2$ which start and end at the point (p,q).

Remark. The mathematical meaning of (2.2) is the original formula (2.1) with a special choice of the approximation of $S(\sigma)$ by Riemann sums.

2.2. The qp-symbol. Let $F_2(p,q,T)$ be the qp-symbol of the evolution operator $U(T)$. In this case instead of formula (1.12), convenient for pq symbols, one should consider the equivalent representation

$$e^{-\frac{i}{\hbar}TH}=\lim_{n\to\infty}\left(e^{-\frac{i\Delta t}{\hbar}V}e^{-\frac{i\Delta t}{\hbar}H_0}\right)^n. \tag{2.3}$$

The distributional kernel $\tilde{K}\left(q',q;\Delta t\right)$ of the operator $e^{-\frac{i\Delta t}{\hbar}V}e^{-\frac{i\Delta t}{\hbar}H_0}$ is given by

$$\tilde{K}\left(q',q;\Delta t\right)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}e^{\frac{i}{\hbar}\left(p(q'-q)-\left(\frac{p^2}{2m}+V(q')\right)\Delta t\right)}dp \tag{2.4}$$

and as in Section 1.2 we obtain

$$K\left(q',t';q,t\right)=\lim_{n\to\infty}\int_{\mathbb{R}^{n-1}}...\prod_{k=0}^{n-1}\tilde{K}\left(q_{k+1},q_k;\Delta t\right)\prod_{k=1}^{n-1}dq_k \tag{2.5}$$

$=\lim_{n\to\infty}\int_{\mathbb{R}^{2n-1}}...\int\exp\left\{\frac{i}{\hbar}\sum_{k=0}^{n-1}\left(p_k\left(q_{k+1}-q_k\right)-H_{\mathrm{c}}\left(p_k,q_{k+1}\right)\Delta t\right)\right\}\frac{dp_0}{2\pi\hbar}\prod_{k=1}^{n-1}\frac{dp_kdq_k}{2\pi\hbar}$.
Using formula (3.19) in Section 3.3 of Chapter 2, we get from (2.5),

$$F_2(p,q,T)=\int_{-\infty}^{\infty}K(q,T;q+v,0)e^{\frac{i}{\hbar}pv}dv \tag{2.6}$$

$=\lim_{n\to\infty}\int_{\mathbb{R}^{2n-2}}\cdots\int\exp\left\{\frac{i}{\hbar}\sum_{k=0}^{n-1}\left(p_k\left(q_{k+1}-q_k\right)-H_{\mathrm{c}}\left(p_k,q_{k+1}\right)\Delta t\right)\right\}\prod_{k=1}^{n-1}\frac{dp_{k-1}dq_k}{2\pi\hbar}$,
where $p_0=p$ and $q_0=q_n=q$. Formula (2.6) can also be obtained from the composition formula

for qp-symbols (see Problem 3.10 in Section 3.4 of Chapter 2) by observing that the qp-symbol of the operator $e^{-\frac{i\Delta t}{\hbar}V}e^{-\frac{i\Delta t}{\hbar}H_0}$ is again $e^{-\frac{i\Delta t}{\hbar}H_c(p,q)}$. In the same spirit as (1.15), formula (2.6) can be written
as the following Feynman path integral for the qp-symbol:

$$F_2(p,q,T)=\int_{\Omega_{(p,q)}(\mathbb{R}^2)}e^{\frac{i}{\hbar}S(\sigma)}\mathscr{D}p\mathscr{D}q \tag{2.7}$$

This expression looks exactly like (2.2), so that the formal path integral representation does not distinguish between pq - and qp-symbols! Of course, the mathematical meaning of (2.7) is the original formula (2.6), which requires a special choice of the approximation of $S(\sigma)$ by Riemann sums, which is different from the one used for the pq-symbol.

Problem 2.1. Deduce formula (2.6) from the composition formula for qp-symbols.

2.3. The Weyl symbol. Let $F(p,q;T)$ be the Weyl symbol of the evolution operator $U(T)$. It follows from the Weyl inversion formula - formula (3.12) in Section 3.3 of Chapter 2 - that

$$F(p,q,T)=\int_{-\infty}^{\infty}K\left(q-\frac{1}{2}v,T;q+\frac{1}{2}v,0\right)e^{\frac{i}{\hbar}pv}dv$$

However, for general potentials $V(q)$ one cannot perform integration over v by using either (1.15) or (2.5), and we choose another approach. Namely, denote by $\tilde{U}(\Delta t)$ an operator [3] with the Weyl symbol $e^{-\frac{i}{\hbar}H_c(p,q)\Delta t}$, and suppose that

$$U(T)=\lim_{n\to\infty}\tilde{U}(\Delta t)^n \tag{2.8}$$

Using the composition formula for the Weyl symbols, formula (3.24) in Section 3.3 of Chapter 2, we can express the Weyl symbol as

$$F(p,q,T)=\lim_{n\to\infty}\int_{\mathbb{R}^{4(n-1)}}...\int_k\exp\left\{\frac{i}{\hbar}\left(2\sum_{k=0}^{n-2}\left(\left(p_k-\xi_k\right)\left(\eta_{k+1}-\eta_k\right)\right.\right.\right. \tag{2.9}$$
$$\left.\left.\left.-\left(q_k-\eta_k\right)\left(\xi_{k+1}-\xi_k\right)\right)-\sum_{k=0}^{n-1}H_c\left(p_k,q_k\right)\Delta t\right)\right\}\prod_{k=1}^{n-1}\frac{dp_kdq_kd\xi_{k-1}d\eta_{k-1}}{\pi\hbar}$$

where $\xi_0=p,\eta_0=q$ and $\xi_{n-1}=p_{n-1},\eta_{n-1}=q_{n-1}$. As for formula (1.15), formula (2.9) can be written as the following Feynman path integral for the Weyl symbol:

$$F(p,q,T) \tag{2.10}$$
$$=\int e^{\frac{i}{\hbar}\int_0^T\left\{2(p(t)-\xi(t))\dot{\eta}(t)-2(q(t)-\eta(t))\dot{\xi}(t)-H_c(p(t),q(t))\right\}dt}\mathscr{D}p\mathscr{D}q\mathscr{D}\xi\mathscr{D}\eta,$$

where

$$\mathscr{D}p\mathscr{D}q\mathscr{D}\xi\mathscr{D}\eta=\lim_{n\to\infty}\prod_{k=1}^{n-1}\frac{dp_kdq_kd\xi_{k-1}d\eta_{k-1}}{\pi\hbar}$$

and "integration" goes over the space of real-valued functions $p(t),q(t),\xi(t)$, and $\eta(t)$ on $[0,T]$ satisfying $\xi(0)=p,\eta(0)=q$ and $\xi(T)=p(T),\eta(T)=q(T)$.

Remark. Expression (2.10) looks very different from (2.2) and (2.7). However, the variables $\xi(t)$ and $\eta(t)$ appear only linearly in the exponential in (2.10), and the integration over them

[03] There is no easy way to express it in terms of $e^{-\frac{i\Delta t}{\hbar}H_0}$ and $e^{-\frac{i\Delta t}{\hbar}V}$.

can be performed explicitly. Indeed, using integration by parts (and ignoring subtleties with the boundary terms) we can transform the integral over $\mathscr{D}\xi$ to

$$\int e^{\frac{2i}{\hbar}\int_0^T \xi(t)(\dot{q}(t)-2\dot{\eta}(t))dt}\mathscr{D}\xi$$

which equals the product of delta-functions $\delta(2\dot{\eta}(t)-\dot{q}(t))$ over $[0,T]$ and allows us to replace $2\dot{\eta}(t)$ by $\dot{q}(t)$ in (2.10). Thus we obtain the formula

$$F(p,q,T)=\int e^{\frac{i}{\hbar}\int_0^T (p\dot{q}-H_c(p,q))dt}\mathscr{D}p\mathscr{D}q$$

which looks exactly like (2.2) and (2.7)! This heuristic argument shows that the Feynman path integral, understood naively, "erases" the difference between various symbols of the evolution operator. Of course, one should always specify particular finite-dimensional approximation of $S(\sigma)$ in order to get correct results.

Problem 2.2. Find the integral kernel of the operator $\tilde{U}(\Delta t)$.

Problem 2.3. Derive formula (2.9).

2.4. The Wick symbol. Instead of the variables $\bar{z}$ and z, used in Section 2.7 of Chapter 2 , it is convenient to use variables $\bar{a}=\sqrt{\hbar}\bar{z}$ and $a=\sqrt{\hbar}z$, which introduce explicit $\hbar$-dependence in the calculus of Wick symbols. Let $H(\bar{a},a)$ be the Wick symbol of a Hamiltonian operator H. Here we derive a formula for the Wick symbol $U(\bar{a},a;T)$ of the evolution operator $U(T)=e^{-\frac{i}{\hbar}TH}$. Denote by $\tilde{U}(\Delta t)$ an operator with the Wick symbol $e^{-\frac{i}{\hbar}H(\bar{a},a)\Delta t}$, and as in the previous section, suppose that

$$U(T)=\lim_{n\to\infty}\tilde{U}(\Delta t)^n \tag{2.11}$$

Using the formula for the composition of Wick symbols (see Theorem 2.2 and Problem 2.18 in Section 2.7 of Chapter 2), we get the following expression
for the Wick symbol $U_n(\bar{a},a;T)$ of the operator $\tilde{U}(\Delta t)^n$:

$$U_n(\bar{a},a;T)=\int\cdots\int\exp\left\{\frac{1}{\hbar}\left(\bar{a}\left(a_{n-1}-a\right)-iH\left(\bar{a},a_{n-1}\right)\Delta t\right.\right. \tag{2.12}$$
$$\left.\left.+\sum_{k=1}^{n-1}\left(\bar{a}_k\left(a_{k-1}-a_k\right)-iH\left(\bar{a}_k,a_{k-1}\right)\Delta t\right)\right)\right\}\prod_{k=1}^{n-1}\frac{d^2a_k}{\pi\hbar},$$

where $a_0=a$. Setting $\bar{a}_n=\bar{a}$, we can rewrite the sum in (2.12) as

$$\sum_{k=1}^{n}\left(\bar{a}_k\left(a_{k-1}-a_k\right)+\bar{a}\left(a_n-a\right)-iH\left(\bar{a}_k,a_{k-1}\right)\Delta t\right),$$

and obtain

$$U(\bar{a},a;T)=\lim_{n\to\infty}U_n(\bar{a},a;T)=\lim_{n\to\infty}\int\cdots\int \tag{2.13}$$
$$\exp\left\{\frac{1}{\hbar}\left(\sum_{k=1}^{n}\left(\bar{a}_k\left(a_{k-1}-a_k\right)+\bar{a}\left(a_n-a\right)-iH\left(\bar{a}_k,a_{k-1}\right)\Delta t\right)\right)\right\}\prod_{k=1}^{n-1}\frac{d^2a_k}{\pi\hbar}.$$

As in the previous examples, we can represent formula (2.13) by the following Feynman path integral for the Wick symbol:

$$U(\bar{a},a;T)=\int\limits_{\left\{\begin{array}{l}\bar{a}(T)=\bar{a}\\ a(0)=a\end{array}\right\}} e^{\frac{i}{\hbar}\int_0^T(i\bar{a}\dot{a}-H(\bar{a},a))dt+\frac{1}{\hbar}\bar{a}(a(T)-a)}\mathscr{D}\bar{a}\mathscr{D}a, \tag{2.14}$$

where

$$\mathscr{D}\bar{a}\mathscr{D}a=\lim_{n\to\infty}\prod_{k=1}^{n-1}\frac{d^2a_k}{\pi\hbar}.$$

Here integration goes over all complex-valued functions $a(t)$ and $\bar{a}(t)$ satisfying boundary conditions $a(0)=a$ and $\bar{a}(T)=\bar{a}$, and such that $\bar{a}(t)$ is complex-conjugated to $a(t)$ for $0<t<T$.

Remark. It should be emphasized that in (2.14) the values $\bar{a}(0)$ and $a(T)$ are not complex-conjugated to the fixed boundary values $a(0)=a$ and $\bar{a}(T)=\bar{a}$, but rather are "variables of integration". This should be compared with formula (1.17), where the boundary values for the function $q(\tau)$ are fixed, and the boundary values for the function $p(\tau)$ are free. The difference is that at $t=0$ we fix the boundary value of the function $a(t)$, while at $t=T$ we fix the boundary value of another function $\bar{a}(t)$.

Remark. The Wick symbol $U(\bar{a},a;-iT)$ of the operator $e^{-\frac{1}{\hbar}TH}=U(-iT)$ can also be represented by

$$\begin{array}{c}U(\bar{a},a;-iT)=\lim\limits_{n\to\infty}U_n(\bar{a},a;-iT)=\lim\limits_{n\to\infty}\int_{\mathbb{C}^{n-1}}\cdots\int\\ \exp\left\{\frac{1}{\hbar}\left(\sum\limits_{k=1}^{n}\left(\bar{a}_k\left(a_{k-1}-a_k\right)-H\left(\bar{a}_k,a_{k-1}\right)\Delta t\right)+\bar{a}\left(a_n-a\right)\right)\right\}\prod\limits_{k=1}^{n-1}\frac{d^2a_k}{\pi\hbar}\\ =\int\limits_{\substack{\bar{a}(T)=\bar{a}\\ a(0)=a}}e^{-\frac{1}{\hbar}\int_0^T(\bar{a}\dot{a}+H(\bar{a},a))dt+\frac{1}{\hbar}\bar{a}(a(T)-a)}\mathscr{D}\bar{a}\mathscr{D}a,\end{array} \tag{2.15}$$

which is the so-called Euclidean path integral - the Feynman path integral with respect to the Euclidean time, which will be discussed in Section 2.3 of Chapter 6. In particular, if the Hamiltonian H has a pure point spectrum and $e^{-\frac{1}{\hbar}TH}$ is of trace class, then using the relation between the trace and Wick symbols (see Problem 2.17 in Section 2.7 of Chapter 2), we obtain from (2.15)

$$\operatorname{Tr}e^{-\frac{1}{\hbar}TH}=\int\limits_{\substack{\bar{a}(0)=\bar{a}(T)\\ a(0)=a(T)}}e^{-\frac{1}{\hbar}\int_0^T(\bar{a}\dot{a}+H(\bar{a},a))dt}\mathscr{D}\bar{a}\mathscr{D}a, \tag{2.16}$$

where now integration goes over all complex-conjugate functions $a(t)$ and $\bar{a}(t)$ satisfying periodic boundary conditions $a(0)=a(T)$ and $\bar{a}(0)=\bar{a}(T)$, and

$$\mathscr{D}\bar{a}\mathscr{D}a=\lim_{n\to\infty}e^{-\frac{1}{\hbar}\bar{a}_na_n}\prod_{k=1}^{n}\frac{d^2a_k}{\pi\hbar}.$$

Indeed, it follows from the identity

$$\begin{array}{c}\sum\limits_{k=1}^{n-1}\bar{a}_k\left(a_{k-1}-a_k\right)+\bar{a}\left(a_{n-1}-a\right)\\ -\ a_k)+\left(\bar{a}_{k+1}-\bar{a}_k\right)a_k\}+\frac{1}{2}\left\{\bar{a}\left(a_{n-1}-a\right)+\left(\bar{a}_1-\bar{a}\right)a\right\}\end{array} \tag{2.17}$$

that when $\bar{a}$ and a are variables of integration, one can put $a_n = a$ and $\bar{a}_0 = \bar{a}$, which together with $\bar{a}_n = \bar{a}$ and $a_0 = a$ imply periodic boundary conditions. Thus

$$\sum_{k=1}^{n-1} \bar{a}_k \left(a_{k-1} - a_k\right) + \bar{a}\left(a_{n-1} - a\right) = \frac{1}{2}\sum_{k=1}^{n} \left\{\bar{a}_k \left(a_{k-1} - a_k\right) + \left(\bar{a}_{k+1} - \bar{a}_k\right) a_k\right\},$$

which in the limit $n \to \infty$ becomes

$$\frac{1}{2}\int_0^T (-\bar{a}\dot{a} + \dot{\bar{a}}a)dt = -\int_0^T \bar{a}\dot{a}dt$$

due to the periodic boundary conditions.
In the holomorphic representation, the matrix symbol $K(\bar{a}, a; T)$ of the evolution operator plays the role of a propagator $K\left(q', T; q, 0\right)$ in the coordinate representation. Using the relation between matrix and Wick symbols (see Lemma 2.4 in Section 2.7 of Chapter 2), we obtain

$$K(\bar{a}, a; T) = \int_{\left\{\begin{array}{l} \bar{a}(T) = \bar{a} \\ a(0) = a \end{array}\right\}} e^{\frac{i}{\hbar}\int_0^T (i\bar{a}\dot{a} - H(\bar{a},a))dt + \frac{1}{\hbar}\bar{a}a(T)} \mathscr{D}\bar{a}\mathscr{D}a. \tag{2.18}$$

Problem 2.4. Find the relation between the Wick symbol of the evolution operator and the propagator. (Hint: Use the analog of formula (2.45) in Section 2.7 of Chapter 2.)

8.1.3 3. Feynman path integral for the harmonic oscillator

As a first impression, one may think that Feynman path integrals are not very practical. Indeed, they are defined as limits of multiple integrals when the number of integrations goes to infinity, and it seems difficult to evaluate them. In fact, this is not so: Feynman path integrals turned out to be very useful for various computations, and for several important cases they can be evaluated exactly. Here we consider the basic example [4], the Feynman path integral for the harmonic oscillator.
3.1. Gaussian integration. Evaluation of Feynman path integrals simplifies when corresponding finite-dimensional integrals can be computed exactly for every n (or for large enough n). This is the case for the important class of Gaussian integrals.

Lemma 3.1 (Gaussian integration). Let A be a positive-definite, real symmetric $n \times n$ matrix. We have

$$\int_{\mathbb{R}^n} e^{-\frac{1}{2}(A\boldsymbol{q},\boldsymbol{q}) + (\boldsymbol{p},\boldsymbol{q})} d^n\boldsymbol{q} = \frac{\sqrt{(2\pi)^n}}{\sqrt{\det A}} e^{\frac{1}{2}\left(A^{-1}\boldsymbol{p},\boldsymbol{p}\right)} \tag{3.1}$$

where $(,)$ stands for the standard Euclidian inner product in $\mathbb{R}^n$.

Proof. Completing the square we obtain

$$-\frac{1}{2}(A\boldsymbol{q},\boldsymbol{q}) + (\boldsymbol{p},\boldsymbol{q}) = -\frac{1}{2}\left(A\left(\boldsymbol{q} - A^{-1}\boldsymbol{p}\right), \left(\boldsymbol{q} - A^{-1}\boldsymbol{p}\right)\right) + \frac{1}{2}\left(A^{-1}\boldsymbol{p}, \boldsymbol{p}\right)$$

so by the change of variables $\boldsymbol{q} = \boldsymbol{x} + A^{-1}\boldsymbol{p}$ the integral reduces to the standard Gaussian integral $\int_{\mathbb{R}^n} e^{-\frac{1}{2}(A\boldsymbol{x},\boldsymbol{x})} d^n\boldsymbol{x}$, which is evaluated by diagonalizing the matrix A and using the one-dimensional Gaussian integral

$$\int_{-\infty}^{\infty} e^{-\frac{1}{2}ax^2} dx = \sqrt{\frac{2\pi}{a}}, \quad a > 0$$

[04] The simplest case of a free particle provides a trivial example, since the Lie-Kato-Trotter product formula reduces to $e^{iA} = \left(e^{\frac{i}{n}A}\right)^n$, and formula (1.14) gives the same answer as (1.11) for every n.

Formula (3.1) is one of the fundamental mathematical facts which is used in many disciplines, from probability theory to number theory. For applications to quantum mechanics, one needs a version of Lemma 3.1 when the decaying exponential factor is replaced by the oscillating exponential factor, as in (1.10).

Corollary 3.1. Let A be a real, non-degenerate symmetric $n \times n$ matrix. Then

$$\int_{\mathbb{R}^n} e^{\frac{i}{2}(A\boldsymbol{q},\boldsymbol{q})+i(\boldsymbol{p},\boldsymbol{q})} d^n\boldsymbol{q} = e^{\frac{\pi i n}{4}-\frac{\pi i \nu}{2}} \frac{\sqrt{(2\pi)^n}}{\sqrt{|\det A|}} e^{-\frac{i}{2}\left(A^{-1}\boldsymbol{p},\boldsymbol{p}\right)} \tag{3.2}$$

where the integral is understood in the distributional sense as $\lim_{R\to\infty}\int_{|q|\le R}$ and ν is the number of negative eigenvalues of A.

Proof. Formula (3.2) follows from (3.1) by analytic continuation. It also can be proved directly by completing the square, diagonalizing the matrix A, and using the Fresnel integral formula (1.10).

There is also a complex version of Gaussian integration, given by the following analog of Lemma 3.1.

Lemma 3.2 (Gaussian integration in complex domain). Let C be a complex $n \times n$ matrix such that its Hermitian part $\frac{1}{2}(C + C^*)$ is positive-definite. We have

$$\int_{\mathbb{C}^n} e^{-(C\boldsymbol{z},\boldsymbol{z})+(\boldsymbol{a},\boldsymbol{z})+(\boldsymbol{z},\boldsymbol{b})} d^{2n}\boldsymbol{z} = \frac{\pi^n}{\det C} e^{\left(C^{-1}\boldsymbol{a},\boldsymbol{b}\right)} \tag{3.3}$$

where $(,)$ stands for the standard Hermitian inner product in $\mathbb{C}^n$, $\boldsymbol{a},\boldsymbol{b} \in \mathbb{C}^n$, and $d^{2n}\boldsymbol{z} = d^2z_1...d^2z_n$.

Problem 3.1. Prove Lemma 3.2.

3.2. Propagator of the harmonic oscillator. The classical harmonic oscillator with one degree of freedom is described by the Lagrangian function $L(q,\dot{q}) = \frac{1}{2}m\left(\dot{q}^2 - \omega^2 q^2\right)$. The corresponding Hamiltonian operator for a quantum harmonic oscillator is given by

$$H = \frac{P^2}{2m} + \frac{m\omega^2 Q^2}{2}$$

The following result is an exact computation of the propagator $K\left(q',t';q,t\right)$ for the harmonic oscillator, using the Feynman path integral in configuration space.

Proposition 3.1. The Feynman path integral for the harmonic oscillator is explicitly evaluated as follows:

$$\int_{P(\mathbb{R})_{q,t}^{q',t'}} e^{\frac{im}{2\hbar}\int_t^{t'}\left(\dot{q}^2-\omega^2q^2\right)d\tau}\mathscr{D}q = \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}\, e^{\frac{im\omega}{2\hbar\sin\omega T}\left\{\left(q^2+q'^2\right)\cos\omega T-2qq'\right\}}$$

where for $\frac{\pi\nu}{\omega} = T_\nu < T < T_{\nu+1} = \frac{\pi(\nu+1)}{\omega}$, $\nu \in \mathbb{N}$, we have

$$\sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}} = e^{-\frac{\pi i}{4}-\frac{\pi i\nu}{2}}\sqrt{\frac{m\omega}{2\pi\hbar|\sin\omega T|}}$$

When $T \to T_\nu$, the right-hand side converges in the distributional sense to $e^{-\frac{\pi i\nu}{2}}\delta\left(q-q'\right)$ for even ν, and to $e^{-\frac{\pi i\nu}{2}}\delta\left(q+q'\right)$ for odd ν.

Proof. In this case the $(n-1)$-fold integral in (1.19) is Gaussian and can be computed exactly using (3.2). Namely, we have

$$\sum_{k=0}^{n-1}\left(\left(q_{k+1}-q_k\right)^2 - \varepsilon^2 q_k^2\right) = \left(A_{n-1}\boldsymbol{q},\boldsymbol{q}\right) - 2(\boldsymbol{p},\boldsymbol{q}) + q^2 + q'^2$$

where $\varepsilon = \omega\Delta t, \boldsymbol{q} = (q_1, ..., q_{n-1}), \boldsymbol{p} = (q, 0, ..., 0, q')$ are vectors in $\mathbb{R}^{n-1}$, and A_{n-1} is the following three-diagonal $(n-1) \times (n-1)$ matrix:

$$A_{n-1} = \begin{pmatrix} 2-\varepsilon^2 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2-\varepsilon^2 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2-\varepsilon^2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2-\varepsilon^2 & -1 \\ 0 & 0 & 0 & \cdots & -1 & 2-\varepsilon^2 \end{pmatrix}$$

It follows from (3.2) that

$$\begin{aligned} &\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{n}{2}} \int_{\mathbb{R}^{n-1}} e^{\frac{im}{2\hbar\Delta t}\sum_{k=0}^{n-1}\left((q_{k+1}-q_k)^2 - \varepsilon^2 q_k^2\right)} \\ &\prod_{k=1}^{n-1} dq_k \\ &= e^{-\frac{\pi i\nu}{2}} \sqrt{\frac{m}{2\pi i\hbar\Delta t\,|\det A_{n-1}|}}\, e^{\frac{im}{2\hbar\Delta t}\left\{q^2+q'^2-\left(A_{n-1}^{-1}p,p\right)\right\}}, \end{aligned} \tag{3.4}$$

where $\nu = \nu_{n-1}$ is the number of negative eigenvalues of the matrix A_{n-1}. It is easy to find $\det A_{n-1}$ and $(A_{n-1}\boldsymbol{p}, \boldsymbol{p})$. Namely, put $a_n = \det A_n$. Expanding $\det A_n$ with respect to the last row, we obtain the three-term recurrence relation

$$a_{n+1} = \left(2-\varepsilon^2\right) a_n - a_{n-1}, \quad n = 0, 1, 2, ..., \tag{3.5}$$

with the initial conditions $a_{-1} = 0$ and $a_0 = 1$. Recurrence relation (3.5) has two linearly independent solutions z^n and z^{-n}, where $2-\varepsilon^2 = z + z^{-1}$, and a solution a_n satisfying these initial conditions is given by

$$a_n = \frac{z^{n+1} - z^{-n-1}}{z - z^{-1}}.$$

From here it is easy to obtain that the eigenvalues of the matrix A_n are given by

$$\lambda_k = z + z^{-1} - 2\cos\frac{\pi k}{n+1}, \quad k = 1, ..., n$$

Since $\varepsilon = \frac{\omega T}{n}$ we have $z = e^{i\theta}$ where $\theta = \varepsilon + O\left(n^{-2}\right)$ and

$$\det A_{n-1} = \frac{\sin n\theta}{\sin\theta} = \frac{\sin\omega T}{\omega\Delta t}\left(1 + O\left(n^{-1}\right)\right) \quad \text{as} \quad n \to \infty,$$

and for n large enough the matrix A_{n-1} has exactly ν negative eigenvalues whenever $T_\nu < T < T_{\nu+1}$. In order to evaluate the inner product $(A_{n-1}\boldsymbol{p}, \boldsymbol{p})$ we only need to know the corner elements of the inverse matrix $B = A_{n-1}^{-1}$, which are given by

$$B_{11} = B_{n-1n-1} = \frac{a_{n-2}}{a_{n-1}} = \frac{\sin(n-1)\theta}{\sin n\theta}, \quad B_{1n-1} = B_{n-11} = \frac{1}{a_n} = \frac{\sin n\theta}{\sin\theta}.$$

Thus we get
$q^2 + q'^2 - \left(A_{n-1}^{-1}\boldsymbol{p}, \boldsymbol{p}\right) = \frac{1}{\sin n\theta}\left(2\sin\frac{\theta}{2}\cos\frac{(2n-1)\theta}{2}\left(q^2+q^2\right) - 2\sin\theta qq'\right)$.
Using these formulas and passing to the limit $n \to \infty$ in (3.4), we obtain the expression for the

propagator for the case $T \neq T_\nu$. The limit $T \to T_\nu$ is evaluated by using the following standard formula in the theory of distributions:

$$\lim_{t\to 0} \frac{1}{\sqrt{2\pi t}} e^{\frac{i(x-y)^2}{2t}} = e^{\frac{\pi i}{4}} \delta(x-y)$$

Remark. It follows from Proposition 3.1 that in the limit $\omega \to 0$ the propagator of the harmonic oscillator turns into the propagator (1.11) of a free particle.

Remark. For even ν, special values T_ν are integer multiples of the period $\frac{2\pi}{\omega}$ of the harmonic oscillator (see Section 1.5 in Chapter 1), so when $t' - t = \widetilde{T}_\nu$, the extremal connecting q at time t and q' at time t' exists if and only if $q' = q$. Correspondingly, when $t' - t = T_\nu$ for odd ν, the extremal connecting q and q' exists if and only if $q' = -q$. For the general case $t' - t \neq T_\nu$, the extremal connecting q at time t and q' at time t' exists for all q and q'. The integer ν is the Morse index of the trajectory $q(\tau)$ - the number of negative eigenvalues of the corresponding Jacobi operator $\mathcal{J}$,

$$\mathcal{J} = -m\frac{d^2}{d\tau^2} - m\omega^2, \quad t \leq \tau \leq t'$$

with Dirichlet boundary conditions (see Problem 1.7 in Section 1.3 in Chapter 1).

Problem 3.2. Compute Weyl, pq, and qp-symbols of the evolution operator for the harmonic oscillator by using: (a) formula (3.2) and path integral representations from Section 2; (b) formula (3.6) and formulas (3.12), (3.18) and (3.19) in Section 3.3 of Chapter 2.

Problem 3.3. Show that the matrix symbol of the evolution operator for the harmonic oscillator is $K(\bar{a}, a; T) = \exp\left\{\bar{a}ae^{-i\omega T} - \frac{i}{2}\omega T\right\}$ by using: (a) series (1.8) in holomorphic representation; (b) Lemma 3.2 and path integral representation from Section 2; (c) formula (3.6) and result of Problem 2.4.

3.3. Mehler identity. It is instructive to compare the closed expression

$$K\left(q', t'; q, t\right) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega T}} e^{\frac{im\omega}{2\hbar \sin \omega T}\left\{\left(q^2+q'^2\right)\cos \omega T - 2qq'\right\}} \tag{3.6}$$

for the propagator of the harmonic oscillator with the series (1.8). Putting $x = \sqrt{\frac{m\omega}{\hbar}}q, y = \sqrt{\frac{m\omega}{\hbar}}q'$ and using the explicit formula for the normalized eigenfunctions

$$\psi_n(q) = \sqrt[4]{\frac{m\omega}{\pi\hbar}} \frac{1}{\sqrt{2^n n!}} e^{-\frac{m\omega}{2\hbar}q^2} H_n(x)$$

corresponding to the eigenvalues $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$, where $H_n(q)$ are classical Hermite-Tchebyscheff polynomials (see Section 2.6 in Chapter 2), we obtain the series

$$K\left(q', t'; q, t\right) = \sqrt{\frac{m\omega}{\pi\hbar}} \sum_{n=0}^{\infty} \frac{e^{-\frac{m\omega}{2\hbar}\left(q^2+q'^2\right) - i\omega T\left(n+\frac{1}{2}\right)}}{2^n n!} H_n(x) H_n(y)$$

which converges in the distributional sense. Setting $z = e^{-i\omega T}$ and comparing with (3.6), we get the formula

$$\sum_{n=0}^{\infty} \frac{z^n}{2^n n!} H_n(x) H_n(y) = \frac{1}{\sqrt{1-z^2}} \exp\left\{\frac{2xyz - \left(x^2+y^2\right)z^2}{1-z^2}\right\} \tag{3.7}$$

where $z \neq \pm 1$, and the square root in the right-hand side is understood as in Proposition 3.1. When $|z| < 1$, formula (3.7) is the classical Mehler identity from the theory of Hermite-Tchebyscheff polynomials. Thus we obtained a distributional form of the Mehler identity for $|z| = 1$ by computing the propagator of the harmonic oscillator in two different ways.

Formula (3.6) shows that the propagator $K(q',t';q,t)$ is a smooth function of q,q' and $T=t'-t$ whenever $T\neq T_\nu$, and it is singular at $T=T_\nu$. Corresponding eigenvalues of the evolution operator $U(T_\nu)$ are $e^{-\pi i\nu\left(n+\frac{1}{2}\right)}$, so that when ν is even we have $U(T_\nu)=e^{-\frac{\pi i\nu}{2}}I$, and therefore

$$K(q',t+T_\nu;q,t)=e^{-\frac{\pi i\nu}{2}}\delta(q-q')$$

in perfect agreement with Proposition 3.1. For odd ν using the series (1.8) we obtain

$$e^{-\frac{i}{\hbar}HT_\nu}=e^{-\frac{\pi i\nu}{2}}\sum_{n=0}^{\infty}(-1)^nP_n$$

where P_n are projection operators on the eigenspaces $\mathbb{C}\psi_n$ of H. Since $H_n(-q)=(-1)^nH_n(q)$, in this case we have

$$K(q',t+T_\nu;q,t)=e^{-\frac{\pi i\nu}{2}}\delta(q+q')$$

which again agrees with Proposition 3.1.

8.1.4 4. Gaussian path integrals

It was already mentioned in Section 1 that in the semi-classical limit $\hbar\to 0$ the leading contribution to the propagator $K(q,t';q,t)$ is given by the classical trajectory $q_{\rm cl}(\tau)$. This suggests to represent the paths $\gamma=q(\tau)\in P(\mathbb{R})_{q,t}^{q',t'}$ as $q(\tau)=q_{\rm cl}(\tau)+y(\tau)$, where $y(\tau)$ - the quantum fluctuation part - satisfies Dirichlet boundary conditions $y(t)=y(t')=0$. It follows from the principle of the least action (see Section 1.2 in Chapter 1) that

$$S(q_{\rm cl}+y)=S_{\rm cl}+\frac{1}{2}\int_t^{t'}\left(m\dot{y}^2-V''(q_{\rm cl}(\tau))\,y^2\right)d\tau+\text{ higher order terms in }y \tag{4.1}$$

where $S_{\rm cl}=S(q_{\rm cl})$ is the classical action. Similarly, for the case of several degrees of freedom,

$$S(\boldsymbol{q}_{\rm cl}+\boldsymbol{y})=S_{\rm cl}+\frac{1}{2}\int_t^{t'}\mathcal{J}(\boldsymbol{y})\boldsymbol{y}d\tau+\text{ higher order terms in }\boldsymbol{y} \tag{4.2}$$

where $\mathcal{J}$ is the corresponding Jacobi operator (see Problem 1.7 in Section 1.3 of Chapter 1). It is remarkable that the Gaussian path integral

$$\int_{\left\{\begin{array}{l}y(t')=0\\ y(t)=0\end{array}\right\}}e^{\frac{im}{2\hbar}\int_t^{t'}\mathcal{J}(\boldsymbol{y})\boldsymbol{y}d\tau}\mathscr{D}\boldsymbol{y} \tag{4.3}$$

over the fluctuating part can be evaluated explicitly in terms of the regularized determinant of the second order differential operator $\mathcal{J}$. Here we do this calculation for the case of the free particle and harmonic oscillator, and give another interpretation of formulas (1.11) and (3.6) for the propagators. The Gaussian path integral (4.3) also plays a fundamental role in the semi-classical asymptotics which we discuss in Section 6.1. In general, formula (4.2), with higher order terms in $\boldsymbol{y}$, and Gaussian integration over $\mathscr{D}\boldsymbol{y}$, constitute a basis for the perturbative expansion of the propagator.

4.1. Gaussian path integral for a free particle. The propagator of a free quantum particle is and the corresponding classical trajectory is

$$q_{\rm cl}(\tau)=q+(\tau-t)\frac{q'-q}{T},\quad T=t'-t$$

Using the decomposition $q(\tau) = q_{\rm cl}(\tau) + y(\tau)$, where $y(t) = y(t') = 0$, we obtain

$$S(q) = \frac{1}{2}\int_t^{t'} m\dot{q}^2 d\tau = S_{\rm cl} + S(y)$$

where

$$S_{\rm cl} = \frac{1}{2}\int_t^{t'} m\dot{q}_{\rm cl}^2 d\tau = \frac{m\,(q-q')^2}{2T}$$

Assuming that $\mathscr{D}q = \mathscr{D}y$ under the "change of variable" $q = q_{\rm cl} + y$, we can rewrite the Feynman path integral for a free particle as

$$K\,(q',t';q,t) = e^{\frac{i}{\hbar}S_{\rm cl}} \int_{\substack{y(t')=0\\ y(t)=0}} e^{\frac{im}{2\hbar}\int_t^{t'}\dot{y}^2 d\tau}\mathscr{D}y.$$

Remarkably, the classical contribution $e^{\frac{i}{\hbar}S_{\rm cl}} = e^{\frac{im(q-q')^2}{2\hbar T}}$ exactly reproduces the exponential factor in the propagator for a free particle. The integral over the fluctuating part - the Gaussian path integral for a free particle - does not depend on q and q' and, as we know, coincides with the prefactor in (4.4).

A more conceptual way to interpret this result is the following. Let

$$A = -D^2, \quad D = \frac{d}{d\tau},$$

be the second order differential operator on the interval $[t,t']$ with Dirichlet boundary conditions $y(t) = y\,(t') = 0$. The operator A is self-adjoint on $L^2\,(t,t')$. For any real-valued, absolutely continuous function $y(\tau)$ satisfying Dirichlet boundary conditions and $y, \dot{y} \in L^2\,(t,t')$, we have by using integration by parts

$$(Ay,y) = -\int_t^{t'} \ddot{y}y d\tau = \int_t^{t'} \dot{y}^2 d\tau$$

The "integrand" in the fluctuation factor

$$\int_{\left\{\begin{array}{l} y\,(t') = 0 \\ y(t) = 0 \end{array}\right\}} e^{\frac{im}{2\hbar}\int_t^{t'}\dot{y}^2 d\tau}\mathscr{D}y$$

is the exponent of the quadratic form of the operator A, and in accordance with the finite-dimensional formula (3.1) it is natural to expect that this Gaussian path integral is proportional to $(\det A)^{-\frac{1}{2}}$. Of course, the problem here is to understand what we mean by a determinant of a differential operator. Clearly, it should be defined by some regularization of the divergent infinite product $\prod_{n=1}^{\infty}\lambda_n$, where λ_n are non-zero eigenvalues of A.

The most natural and useful regularization is given by the so-called operator zeta-function. Namely, let A be a non-negative self-adjoint operator in the Hilbert space $\mathscr{H}$ with pure point spectrum $0 \le \lambda_1 \le \lambda_2 \le \ldots$, such that for some $\alpha > 0$ the operator $(A+I)^{-\alpha}$ is of trace class. Then the zetafunction $\zeta_A(s)$ of the operator A is defined for $\mathrm{Re}\,s > \alpha$ by the following absolutely convergent series:

$$\zeta_A(s) = \sum_{\lambda_n > 0} \frac{1}{\lambda_n^s}.$$

If $\zeta_A(s)$ admits a meromorphic continuation to a larger domain containing the point $s = 0$ and is regular at $s = 0$, then we define a regularized determinant of A by

$$\det' A = \exp\left\{-\frac{d\zeta_A}{ds}(0)\right\} \tag{4.5}$$

Here the prime on the symbol det indicates that zero eigenvalues are excluded from the definition of an operator zeta-function. In the special case when 0 is not the eigenvalue of A, it is customary to denote the regularized
determinant of A by $\det A$. We will also write

$$\det' A = \prod_{\lambda_n>0}{}' \lambda_n$$

where the prime indicates that the infinite product is regularized by the operator zeta-function. We have $\zeta_{cA}(s) = c^{-s}\zeta_A(s)$ for $c > 0$, so that

$$\det' cA = c^{\zeta_A(0)} \det' A$$

which shows that $\zeta_A(0)$ plays the role of "regularized scaling dimension" of the Hilbert space $\mathscr{H}$ (with respect to the operator A). When $\dim_{\mathbb{C}} \mathscr{H} = n < \infty$ and $A > 0$, then $\zeta_A(0) = n$ and $\zeta'_A(0) = \log\lambda_1 + \cdots + \log\lambda_n$, and we recover the usual definition of $\det A$.

This basic outline works for the general case of elliptic operators on a compact manifold M. In quantum mechanics, only determinants of differential operators on one-dimensional [5] manifolds $M = [t, t']$ or $M = S^1$ appear. Their systematic study will be presented in Section 5 , while here we consider the simplest case of the second derivative operator $A = -D^2$ associated with a free particle. The corresponding eigenvalues of A are $\lambda_n = \left(\frac{\pi n}{T}\right)^2$, $n = 1, 2, ...$, and we have for the operator zeta-function

$$\zeta_A(s) = \left(\frac{T}{\pi}\right)^{2s} \zeta(2s)$$

where $\zeta(s)$ is the Riemann zeta-function. Using classical formulas $\zeta(0) = -\frac{1}{2}$ and $\zeta'(0) = -\frac{1}{2}\log 2\pi$, we obtain

$$\zeta_A(0) = -\frac{1}{2} \quad \text{and} \quad \zeta'_A(0) = -\log\frac{T}{\pi} - \log 2\pi = -\log 2T \tag{4.6}$$

Thus for the operator $A = -D^2$ on the interval $[t, t']$ with Dirichlet boundary conditions we have

$$\det A = 2T \tag{4.7}$$

The formula

$$\int_{\left\{\begin{array}{c} y(t') = 0 \\ y(t) = 0 \end{array}\right\}} e^{\frac{im}{2\hbar}\int_t^{t'} \dot{y}^2 d\tau} \mathscr{D}y = \sqrt{\frac{m}{2\pi i\hbar T}}$$

agrees with our interpretation that the Gaussian path integral is proportional to $(\det A)^{-\frac{1}{2}}$. The coefficient of proportionality $c_{m,\hbar} = \sqrt{\frac{m}{\pi i\hbar}}$ is determined by comparison with the actual propagator for a free particle.

Remark. In Section 3.1 of Chapter 6 we will prove that for Gaussian Wiener integrals the corresponding constant is $\sqrt{\frac{m}{\pi\hbar}}$.

Problem 4.1. Show that the propagator of a particle in a constant uniform field f is given by the following formula:

[05] Higher-dimensional manifolds are used in quantum field theory.

$$K(q',t';q,t)=\sqrt{\frac{m}{2\pi i\hbar T}}e^{\frac{i}{2\hbar}\left\{\frac{m(q-q')^2}{T}+fT(q+q')-\frac{f^2T^3}{12m}\right\}}.$$

(Hint: Use Lagrangian function $L=\frac{1}{2}m\dot{q}^2+fq$.)

4.2. Gaussian path integral for the harmonic oscillator. It is remarkable that the same interpretation (with the same constant $c_{m,\hbar}$) holds for the harmonic oscillator. Namely, according to Proposition 3.1 we have

$$\begin{aligned}K(q',t';q,t)&=\int_{P(\mathbb{R})^{q,t}_{q,t}}e^{\frac{im}{2\hbar}\int_t^{t'}\left(\dot{q}^2-\omega^2q^2\right)d\tau}\mathscr{D}q\\&=\sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}\exp\left\{\frac{im\omega}{2\hbar\sin\omega T}\left(\left(q^2+q^2\right)\cos\omega T-2qq'\right)\right\}.\end{aligned}$$

Now solving classical equations of motion with the boundary conditions $q(t)=q$ and $q(t')=q'$, we readily compute that for $T\neq T_\nu$,

$$S_{\mathrm{cl}}=\frac{m}{2}\int_t^{t'}\left(\dot{q}_{\mathrm{cl}}^2-\omega^2q_{\mathrm{cl}}^2\right)d\tau=\frac{m\omega}{2\sin\omega T}\left(\left(q^2+q'^2\right)\cos\omega T-2qq'\right)$$

so that $e^{\frac{i}{\hbar}S_{\mathrm{cl}}}$ is exactly the exponential factor in the propagator. For the fluctuating factor - the Gaussian path integral for the harmonic oscillator - we have

$$\int_{\left\{\begin{array}{c}y(t')=0\\y(t)=0\end{array}\right\}}e^{\frac{im}{2\hbar}\int_t^{t'}\left(\dot{y}^2-\omega^2y^2\right)d\tau}\mathscr{D}y=\sqrt{\frac{m}{\pi i\hbar\det A_\omega}},$$

where $A_\omega=-D^2-\omega^2$ is the second order differential operator on the interval $[t,t']$ with Dirichlet boundary conditions. Thus to justify, in this case, the interpretation of the fluctuating factor in terms of the regularized determinant, we need to show that $\det A_\omega=\frac{2\sin\omega T}{\omega}$ when $T\neq T_\nu$.

At a heuristic level, this can be done by the following beautiful computation, which goes back to Euler. Namely, the eigenvalues of A_ω are $\lambda_n(\omega)=\left(\frac{\pi n}{T}\right)^2-\omega^2$ (0 is not an eigenvalue for A_ω since $T\neq T_\nu$), and we have

$$\frac{\det A_\omega}{\det A_0}=\prod_{n=1}^{\infty}\frac{\lambda_n(\omega)}{\lambda_n(0)}=\prod_{n=1}^{\infty}\left(1-\frac{\omega^2T^2}{\pi^2n^2}\right)=\frac{\sin\omega T}{\omega T}$$

Since $\det A_0=2T$, we get the result! For the rigorous derivation, it is more convenient to consider the positive-definite operator $A_{i\omega}$, where $\omega>0$, instead of the operator A_ω.

Lemma 4.1. Let $A_{i\omega}=-D^2+\omega^2$ be the second order differential operator on the interval $[t,t']$ with Dirichlet boundary conditions. Then

$$\det A_{i\omega}=\frac{2\sinh\omega T}{\omega}$$

Proof. Denoting $\zeta_{i\omega}(s)=\zeta_{A_{i\omega}}(s)$, we have for $\operatorname{Re}s>\frac{1}{2}$,

$$\begin{aligned}\zeta_{i\omega}(s)&=\frac{1}{\Gamma(s)}\int_0^{\infty}e^{-\omega^2x}\sum_{n=1}^{\infty}e^{-\frac{\pi^2n^2}{T^2}x}x^s\frac{dx}{x}\\&=\frac{1}{2\Gamma(s)}\int_0^{\infty}e^{-\omega^2x}\vartheta\left(\frac{\pi x}{T^2}\right)x^s\frac{dx}{x}-\frac{1}{2\omega^{2s}}\end{aligned}$$

where $\vartheta(x)=\sum_{n\in\mathbb{Z}}e^{-\pi n^2x}$ is the Jacobi theta series. Using the Jacobi inversion formula

$$\vartheta\left(\frac{1}{x}\right)=\sqrt{x}\vartheta(x),\quad x>0$$

we get the following representation:

$$\begin{aligned}\zeta_{i\omega}(s)&=-\frac{1}{2\omega^{2s}}+\frac{T}{2\sqrt{\pi}\Gamma(s)}\int_0^\infty e^{-\omega^2x}\vartheta\left(\frac{T^2}{\pi x}\right)x^{s-\frac{1}{2}}\frac{dx}{x}\\&=-\frac{1}{2\omega^{2s}}+\frac{T\Gamma\left(s-\frac{1}{2}\right)}{2\sqrt{\pi}\omega^{2s-1}\Gamma(s)}+\frac{T}{\sqrt{\pi}\Gamma(s)}\int_0^\infty e^{-\omega^2x}\sum_{n=1}^\infty e^{-\frac{n^2T^2}{x}}x^{s-\frac{1}{2}}\frac{dx}{x}\\(4.8)&=-\frac{1}{2\omega^{2s}}+\frac{T\Gamma\left(s-\frac{1}{2}\right)}{2\sqrt{\pi}\omega^{2s-1}\Gamma(s)}+\frac{2T}{\sqrt{\pi}\Gamma(s)}\sum_{n=1}^\infty\left(\frac{nT}{\omega}\right)^{s-\frac{1}{2}}K_{s-\frac{1}{2}}(2\omega nT),\end{aligned}\tag{4.8}$$

where

$$K_s(x)=\frac{1}{2}\int_0^\infty e^{-\frac{x}{2}\left(u+u^{-1}\right)}u^s\frac{du}{u},x>0$$

is Macdonald's K-function (modified Bessel function of the second kind). Since $K_s(x)=O\left(e^{-x}\right)$ as $x\to\infty$, uniformly in $s\in\mathbb{C}$ on compact subsets, it follows from representation (4.8) and the Weierstrass M-test that $\zeta_{i\omega}(s)$ admits meromorphic continuation to the entire s-plane with simple poles at $s\in-\frac{1}{2}+\mathbb{Z}_{\geq0}$. Since $\lim_{s\to0}s\Gamma(s)=1$, we obtain $\zeta_{i\omega}(0)=-\frac{1}{2}$. Using classical formulas

$$K_{\frac{1}{2}}(x)=K_{-\frac{1}{2}}(x)=\sqrt{\frac{\pi}{2x}}e^{-x}\tag{4.9}$$

and $\Gamma\left(\frac{1}{2}\right)=\sqrt{\pi}$, we obtain from (4.8),

$$\begin{aligned}\frac{d\zeta_{i\omega}}{ds}(0)&=\log\omega-\omega T+\sum_{n=1}^\infty\frac{1}{n}e^{-2n\omega T}\\&=\log\omega-\omega T-\log\left(1-e^{-2\omega T}\right)\end{aligned}$$

so that

$$\det A_{i\omega}=\exp\left\{-\frac{d\zeta_{i\omega}}{ds}(0)\right\}=\frac{2\sinh\omega T}{\omega}$$

Corollary 4.1. Let $B_\omega=-D^2+i\omega D$ be the second order differential operator on the interval $[t,t']$ with Dirichlet boundary conditions. Then $\det B_{2\omega}=\det A_\omega$.

Proof. The substitution $y(\tau)=e^{i\omega\tau}f(\tau)$ transforms the eigenvalue problem $B_{2\omega}y=\lambda y$ to the eigenvalue problem $A_\omega f=\lambda f$.

Let I be the identity operator in $L^2(t,t')$. In addition to the regularized determinant $\det' A$ of the differential operator $A=-D^2$, it is possible to define the so-called characteristic determinant of A - an entire function $\det(A-\lambda I)$ on the complex λ-plane, whose only simple zeros are the eigenvalues $\lambda_n=\left(\frac{\pi n}{T}\right)^2$.

Indeed, for $\operatorname{Re}(\lambda_1-\lambda)>0$ consider the zeta-function

$$\zeta_{A-\lambda I}(s)=\sum_{n=1}^\infty\frac{1}{(\lambda_n-\lambda)^s}=\sum_{n=1}^\infty e^{-s\log(\lambda_n-\lambda)}\tag{4.10}$$

where we are using the principal branch of the logarithm. As before, $\zeta_{A-\lambda I}(s)$ is absolutely convergent for $\operatorname{Re} s > \frac{1}{2}$, admits a meromorphic continuation to the complex s-plane, and is regular at $s = 0$. Thus for $\operatorname{Re}(\lambda_1 - \lambda) > 0$ we define

$$\det(A - \lambda I) = \prod_{n=1}^{\infty} (\lambda_n - \lambda) = \exp\left\{ -\frac{\partial \zeta_{A-\lambda I}}{\partial s}(0) \right\}$$

which is a holomorphic function of λ. Now suppose that $\det(A - \lambda I)$ is already defined for $\operatorname{Re}(\lambda_N - \lambda) > 0$ and is holomorphic. To extend it to the domain $\operatorname{Re}(\lambda_{N+1} - \lambda) > 0$, we set

$$\det(A - \lambda I) = \prod_{k=1}^{N} (\lambda_k - \lambda) \prod_{n=N+1}^{\infty} (\lambda_n - \lambda)$$

where the regularized product is defined by the "truncated" zeta-function

$$\zeta_{A-\lambda I}^{(N+1)}(s) = \sum_{n=N+1}^{\infty} \frac{1}{(\lambda_n - \lambda)^s}$$

as

$$\prod_{n=N+1}^{\infty} (\lambda_n - \lambda) = \exp\left\{ -\frac{\partial \zeta_{A-\lambda I}^{(N+1)}}{\partial s}(0) \right\} \tag{4.11}$$

It requires to prove that $\zeta_{A-\lambda I}^{(N+1)}(s)$ admits a meromorphic continuation to the complex s-plane and is regular at $s = 0$. This is done by using the representation

$$\zeta_{A-\lambda I}^{(N+1)}(s) = \frac{1}{2\Gamma(s)} \int_1^{\infty} e^{-\lambda x} \vartheta_{N+1}(x) x^s \frac{dx}{x} + \frac{1}{2\Gamma(s)} \int_0^1 e^{-\lambda x} \vartheta_{N+1}(x) x^s \frac{dx}{x}$$

where

$$\vartheta_{N+1}(x) = \vartheta(x) - 2 \sum_{n=1}^{N} e^{-\lambda_n x} - 1$$

Since $\operatorname{Re}(\lambda_n - \lambda) > 0$ for all $n > N$, the first integral in this formula is absolutely convergent for all $s \in \mathbb{C}$ and represents a holomorphic function. Using the Jacobi inversion formula and expanding $e^{-\lambda x}, e^{-\lambda_1 x}, \ldots, e^{-\lambda_N x}$ into power series in x, we conclude, just as before, that the second integral admits a meromorphic continuation to the s-plane with simple poles at $s \in -\frac{1}{2} + \mathbb{Z}_{\geq 0}$. Since for $M > N$

$$\prod_{n=N+1}^{\infty} (\lambda_n - \lambda) = \prod_{k=N+1}^{M} (\lambda_k - \lambda) \prod_{n=M+1}^{\infty} (\lambda_n - \lambda)$$

$\det(A - \lambda I)$ is well defined, and is an entire function of λ with simple zeros at $\lambda = \lambda_n$.

To obtain a closed (and simple) formula for $\det(A - \lambda I)$, observe that for $\operatorname{Re}(\lambda_1 - \lambda) > 0$ it follows from (4.10) that

$$\frac{\partial \zeta_{A-\lambda I}}{\partial \lambda}(s) = s \sum_{n=1}^{\infty} \frac{1}{(\lambda_n - \lambda)^{s+1}}$$

This series is absolutely convergent for $\operatorname{Re} s > -\frac{1}{2}$, so that for $\operatorname{Re}(\lambda_1 - \lambda) > 0$ we have

$$\frac{d}{d\lambda} \log \det(A - \lambda I) = -\frac{\partial^2}{\partial s \partial \lambda} \zeta_{A-\lambda I}(0) = \sum_{n=1}^{\infty} \frac{1}{\lambda - \lambda_n} \tag{4.12}$$

By analytic continuation, formula (4.12) is valid for all $\lambda \neq \lambda_n$. Since $\lambda_n = \left(\frac{\pi n}{T}\right)^2$, we have

$$\sum_{n=1}^{\infty} \frac{1}{\lambda - \lambda_n} = \frac{T}{2\sqrt{\lambda}} \cot \sqrt{\lambda} T - \frac{1}{2\lambda}$$

so that

$$\det(A - \lambda I) = c \frac{\sin \sqrt{\lambda} T}{\sqrt{\lambda}}$$

and comparison between formula $\det(A + \omega^2 I) = \det A_{i\omega}$ and Lemma 4.1 gives $c = 2$. Thus we have proved the following result.

Lemma 4.2. The characteristic determinant $\det(A - \lambda I)$ of the operator $A = -D^2$ on the interval $[t, t']$ with Dirichlet boundary conditions is well defined, and is an entire function of λ. It is given explicitly by

$$\det(A - \lambda I) = \det A \prod_{n=1}^{\infty} \left(1 - \frac{\lambda}{\lambda_n}\right) = \frac{2 \sin \sqrt{\lambda} T}{\sqrt{\lambda}}$$

Problem 4.2. Prove the Jacobi inversion formula. (Hint: Use the Poisson summation formula

$$\sum_{n=-\infty}^{\infty} f(n) = \sqrt{2\pi} \sum_{n=-\infty}^{\infty} \hat{f}(2\pi n)$$

where $f \in \mathscr{S}(\mathbb{R})$ and $\hat{f}$ is the Fourier transform of f.)

Problem 4.3. Prove formula (4.9).

Problem 4.4. Let

$$L = \frac{m}{2}\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right) + \frac{eB}{2c}(x\dot{y} - y\dot{x})$$

be the Lagrangian of a classical particle moving in the constant uniform magnetic field $\boldsymbol{B} = (0, 0, B)$. Show that the propagator of the corresponding quantum particle (see Example 2.3 in Section 2.4 of Chapter 2) is given by

$$K(\boldsymbol{r}', t'; \boldsymbol{r}, t) = \left(\frac{m}{2\pi i \hbar T}\right)^{\frac{3}{2}} \frac{\omega T}{\sin \omega T} \exp \frac{im}{2\hbar} \left\{ \frac{(z - z')^2}{T} + \omega \cot \omega T \left[(x - x')^2 + (y - y')^2\right] + 2\omega (xy' - yx') \right\}.$$

(Hint: Use Corollary 4.1.)

8.1.5 5. Regularized determinants of differential operators

Here we study the characteristic determinant $\det(A - \lambda I)$ of the SturmLiouville operator

$$A = -D^2 + u(x), \quad D = \frac{d}{dx}$$

on the interval $[0, T]$ with Dirichlet or periodic boundary conditions, and its generalizations to the matrix case.

5.1. Dirichlet boundary conditions. Suppose that $u(x) \in C^1([0, T], \mathbb{R})$. The operator A is self-adjoint on $L^2(0, T)$ with domain

$$D(A) = \left\{y(x) \in W^{2,2}(0, T) : y(0) = y(T) = 0\right\}$$

where $W^{2,2}(0,T)$ is the Sobolev space. It has a pure point spectrum with simple eigenvalues $\lambda_1 < \lambda_2 < \cdots < \lambda_n < \cdots$, accumulating to ∞. Moreover, as $n \to \infty$,

$$\lambda_n = \frac{\pi^2 n^2}{T^2} + c + O\left(n^{-2}\right), \quad \text{where} \quad c = \frac{1}{T}\int_0^T u(x)dx \tag{5.1}$$

Consider first the case $A > 0$. Putting

$$\vartheta_A(t) = \sum_{n=1}^{\infty} e^{-\lambda_n t}$$

we have for $\operatorname{Re} s > \frac{1}{2}$,

$$\zeta_A(s) = \frac{1}{\Gamma(s)}\int_0^\infty \vartheta_A(t)t^s\frac{dt}{t} \tag{5.2}$$

$$= \frac{1}{\Gamma(s)}\int_1^\infty \vartheta_A(t)t^s\frac{dt}{t} + \frac{1}{\Gamma(s)}\int_0^1 \vartheta_A(t)t^s\frac{dt}{t} \tag{5.3}$$

Since $\vartheta_A(t) = O\left(e^{-\lambda_1 t}\right)$ as $t \to \infty$, the first integral in (5.3) converges absolutely for all $s \in \mathbb{C}$ and represents an entire function. Using asymptotics (5.1) and the Jacobi inversion formula we get as $t \to 0$,

$$\vartheta_A(t) = \frac{1}{2}e^{-ct}\left(\vartheta\left(\frac{\pi t}{T^2}\right) - 1\right)(1 + O(t)) = \frac{a_{-\frac{1}{2}}}{\sqrt{t}} + a_0 + \tilde{\vartheta}_A(t),$$

where

$$a_{-\frac{1}{2}} = \frac{T}{2\sqrt{\pi}}, \quad a_0 = -\frac{1}{2} \tag{5.4}$$

and $\widetilde{\vartheta}_A(t) = O(\sqrt{t})$. Thus for the second integral in (5.3) we have

$$\frac{1}{\Gamma(s)}\int_0^1 \vartheta_A(t)t^s\frac{dt}{t} = \frac{a_{-\frac{1}{2}}}{\left(s-\frac{1}{2}\right)\Gamma(s)} + \frac{a_0}{s\Gamma(s)} + \frac{1}{\Gamma(s)}\int_0^1 \widetilde{\vartheta}_A(t)t^s\frac{dt}{t},$$

so that it admits a meromorphic continuation to the half-plane $\operatorname{Re} s > -\frac{1}{2}$ and is regular at $s = 0$. Therefore we can define

$$\det{}' A = \prod_{n=1}^{\infty}\lambda_n = \exp\left\{-\frac{d\zeta_A}{ds}(0)\right\}$$

Now repeating verbatim the arguments in the proof of Lemma 4.2, we see that for $\operatorname{Re}(\lambda_N - \lambda) > 0$ the truncated zeta-function $\zeta_{A-\lambda I}^{(N+1)}(s)$ admits a meromorphic continuation to $\operatorname{Re} s > -\frac{1}{2}$, and is regular at $s = 0$. Defining the regularized product $\prod_{n=N+1}^{\infty}(\lambda_n - \lambda)$ by the same formula (4.11), we see that

$$\det(A - \lambda I) = \prod_{k=1}^{N}(\lambda_k - \lambda)\prod_{n=N+1}^{\infty}(\lambda_n - \lambda)$$

is an entire function of λ with simple zeros at λ_n. To remove the assumption $A > 0$, replace A by $\tilde{A} = A + (a - \lambda_1)I > 0$, where $a > 0$. Then [6]

$$\det(A - \lambda I) = \det\left(\tilde{A} - (\lambda + \lambda_1 - a)I\right)$$

and

$$\det{}' A = \begin{cases} \det A & \text{if 0 is not an eigenvalue of } A \\ \lim_{\lambda\to 0} \lambda^{-1} \det(A+\lambda I) & \text{if 0 is an eigenvalue of } A \end{cases}$$

Let $y_1(x,\lambda)$ be the solution of the second order differential equation

$$-y'' + u(x)y = \lambda y \tag{5.5}$$

on $[0,T]$, satisfying initial conditions

$$y_1(0,\lambda) = 0, \quad y_1'(0,\lambda) = 1 \tag{5.6}$$

It is known that for every $0 \le x \le T$, the solution $y_1(x,\lambda)$ is an entire function of λ of order $\frac{1}{2}$ and as $\lambda \to \infty$,

$$y_1(x,\lambda) = \frac{\sin\sqrt{\lambda}x}{\sqrt{\lambda}} + O\left(|\lambda|^{-1} e^{|\operatorname{Re}\sqrt{\lambda}|x}\right) \tag{5.7}$$

The entire function $d(\lambda) = y_1(T,\lambda)$ has simple zeros at the eigenvalues λ_n of the operator A, and has the following Hadamard product representation:

$$d(\lambda) = c\lambda^\delta \prod_{\lambda_n \neq 0} \left(1 - \frac{\lambda}{\lambda_n}\right). \tag{5.8}$$

Here c is a constant, $\delta = 1$ if 0 is an eigenvalue of A, and $\delta = 0$ otherwise.

Theorem 5.1. The characteristic determinant $\det(A-\lambda I)$ is given by the simple formula

$$\det(A-\lambda I) = 2d(\lambda)$$

Moreover,

$$\frac{\det(A-\lambda I)}{\det' A} = (-\lambda)^\delta \prod_{\lambda_n \neq 0} \left(1 - \frac{\lambda}{\lambda_n}\right)$$

which fixes the constant in (5.8) as $c = \frac{1}{2}(-1)^\delta \det' A$.

Proof. Since both functions are entire, it is sufficient to prove the equality $\det(A-\lambda I) = 2d(\lambda)$ for $\operatorname{Re}(\lambda_1 - \lambda) > 0$. In this case, using

$$\zeta_{A-\lambda I}(s) = \frac{1}{\Gamma(s)} \int_0^\infty \operatorname{Tr} e^{-(A-\lambda I)t} t^s \frac{dt}{t}$$

for $\operatorname{Re} s > \frac{1}{2}$, and differentiating under the integral sign we get

$$\frac{\partial}{\partial\lambda}\zeta_{\Lambda-\lambda I}(s) = \frac{1}{\Gamma(s)} \int_0^\infty \operatorname{Tr} e^{-(A-\lambda I)t} t^s dt$$

which is now absolutely convergent for $\operatorname{Re} s > -\frac{1}{2}$. Differentiating with respect to s at $s = 0$, we obtain

$$\frac{\partial^2}{\partial s \partial\lambda}\zeta_{A-\lambda I}(0) = \int_0^\infty \operatorname{Tr} e^{-(A-\lambda I)t} dt = \operatorname{Tr}(A-\lambda I)^{-1}$$

It follows from (5.1) that the operator $R_\lambda = (A-\lambda I)^{-1}$ - the resolvent of A - is of trace class. Thus all our manipulations are justified and we arrive at the following very useful formula:

[06] The definition of $\det' A$ does not depend on the choice of $a > 0$.

$$\frac{d}{d\lambda}\log\det(A-\lambda I) = -\operatorname{Tr} R_\lambda \tag{5.9}$$

which generalizes the familiar property of finite-dimensional determinants.
To compute the trace in (5.9), we use the representation of R_λ for $\lambda \neq \lambda_n$ as an integral operator with the continuous kernel $R_\lambda(x,\xi)$ (cf. formula (2.21) in Section 2.2 of Chapter 3). Namely, let $y_2(x,\lambda)$ be another solution of (5.5) with boundary conditions $y_2(T,\lambda)=0$ and $y_2'(T,\lambda)=1$, so that

$$W(y_1,y_2)(\lambda) = y_1'(x,\lambda)y_2(x,\lambda) - y_1(x,\lambda)y_2'(x,\lambda) = -d(\lambda).$$

Using the method of variation of parameters, for the solution of the inhomogeneous equation

$$-y'' + u(x)y = \lambda y + f(x), \quad \lambda \neq \lambda_n,$$

satisfying Dirichlet boundary conditions we get

$$y(x) = \int_0^T R_\lambda(x,\xi)f(\xi)d\xi$$

where

$$R_\lambda(x,\xi) = \begin{cases} -\frac{y_1(x,\lambda)y_2(\xi,\lambda)}{d(\lambda)} & \text{if } x \le \xi \\ -\frac{y_1(\xi,\lambda)y_2(x,\lambda)}{d(\lambda)} & \text{if } x \ge \xi \end{cases} \tag{5.10}$$

Since R_λ is a trace class operator on $L^2(0,T)$ with the integral kernel $R_\lambda(x,\xi)$, which is a continuous function on $[0,T]\times[0,T]$, its operator trace equals the "matrix trace",

$$\operatorname{Tr} R_\lambda = \int_0^T R_\lambda(x,x)dx = -\frac{1}{d(\lambda)}\int_0^T y_1(x,\lambda)y_2(x,\lambda)dx$$

We evaluate the last integral by the same computation used in the proof of Proposition 2.1 in Section 2.1 of Chapter 3. Namely, put $\dot y(x,\lambda) = \frac{\partial y}{\partial\lambda}(x,\lambda)$, and consider the following pair of equations:

$$\begin{aligned} -\dot y_1'' + u(x)\dot y_1 &= \lambda\dot y_1 + y_1, \\ -y_2'' + u(x)y_2 &= \lambda y_2. \end{aligned}$$

Multiplying the first equation by $y_2(x,\lambda)$, the second equation by $\dot y_1(x,\lambda)$ and subtracting, we obtain

$$y_1y_2 = \dot y_1y_2'' - \dot y_1''y_2 = -W(\dot y_1,y_2)'$$

so that

$$\int_0^T y_1(x,\lambda)y_2(x,\lambda)dx = -W(\dot y_1,y_2)\big|_0^T \tag{5.11}$$

This formula is valid for any two solutions of the differential equation (5.5). Using boundary conditions for the solutions y_1 and y_2, we finally get

$$\int_0^T y_1(x,\lambda)y_2(x,\lambda)dx = \dot y_1(T,\lambda) \tag{5.12}$$

Thus we have proved that for $\operatorname{Re}(\lambda_1-\lambda)>0$,

$$\operatorname{Tr} R_\lambda = -\frac{d}{d\lambda}\log d(\lambda) \tag{5.13}$$

which implies that

$$\det(A-\lambda I) = Cd(\lambda) \tag{5.14}$$

for all $\lambda \in \mathbb{C}$ and some constant C.
It follows from (5.7) that

$$d(-\mu) = \frac{e^{\sqrt{\mu}T}}{2\sqrt{\mu}}\left(1+O\left(\mu^{-\frac{1}{2}}\right)\right) \quad \text{as} \quad \mu \to +\infty. \tag{5.15}$$

Thus in order to determine the constant C in (5.14), it is sufficient to compute the asymptotics of $\det(A+\mu I)$ as $\mu \to +\infty$. We have

$$\zeta_{A+\mu I}(s) = \frac{1}{\Gamma(s)}\int_1^\infty \vartheta_A(t)e^{-\mu t}t^s\frac{dt}{t} + \frac{1}{\Gamma(s)}\int_0^1 \vartheta_A(t)e^{-\mu t}t^s\frac{dt}{t}$$

The first integral is an entire function of s whose derivative at $s=0$ exponentially decays as $\mu \to +\infty$. For the second integral we have

$$\begin{aligned}\frac{1}{\Gamma(s)}\int_0^1 \vartheta_A(t)e^{-\mu t}t^s\frac{dt}{t} &= \frac{1}{\Gamma(s)}\int_0^1 \tilde{\vartheta}_A(t)e^{-\mu t}t^s\frac{dt}{t}\\ &\quad + \frac{1}{\Gamma(s)}\int_0^1 \left(\frac{a_{-\frac{1}{2}}}{\sqrt{t}}+a_0\right)e^{-\mu t}t^s\frac{dt}{t}\end{aligned}$$

Since $\widetilde{\vartheta}_A(t) = O(\sqrt{t})$ as $t \to 0$, the first integral is absolutely convergent for $\operatorname{Re} s > -\frac{1}{2}$ and its derivative at $s=0$ is $O\left(\mu^{-\frac{1}{2}}\right)$ as $\mu \to +\infty$. For the
remaining integral we have

$$\begin{aligned}\frac{1}{\Gamma(s)}\int_0^1 \left(\frac{a_{-\frac{1}{2}}}{\sqrt{t}}+a_0\right)e^{-\mu t}t^s\frac{dt}{t} &= \frac{a_{-\frac{1}{2}}\mu^{\frac{1}{2}-s}}{\Gamma(s)}\left(\Gamma\left(s-\frac{1}{2}\right)-\int_\mu^\infty e^{-t}t^{s-\frac{1}{2}}\frac{dt}{t}\right)\\ &\quad + \frac{a_0\mu^{-s}}{\Gamma(s)}\left(\Gamma(s)-\int_\mu^\infty e^{-t}t^s\frac{dt}{t}\right)\end{aligned}$$

It is elementary to show that the s-derivative of this integral at $s=0$ has asymptotics $-2\sqrt{\pi}a_{-\frac{1}{2}}\sqrt{\mu} - a_0\log\mu + O\left(e^{-\mu/2}\right)$ as $\mu \to +\infty$. Using (5.4) we finally obtain

$$\det(A+\mu I) = \frac{e^{\sqrt{\mu}T}}{\sqrt{\mu}}\left(1+O\left(\mu^{-\frac{1}{2}}\right)\right)$$

as $\mu \to +\infty$, and comparison with (5.15) gives $C=2$.
Remark. When zero is not an eigenvalue of A, its inverse A^{-1} is a trace class operator and

$$\frac{\det(A-\lambda I)}{\det A} = \det{}_F\left(I-\lambda A^{-1}\right)$$

where $\det_F$ is the Fredholm determinant.
Remark. In Section 6.1 we will use Theorem 5.1 for evaluating the fluctuating factor in the semi-classical asymptotics of the propagator, and in Section 3.1 of Chapter 6 - for evaluating Gaussian Wiener integrals.

A similar result holds for the matrix-valued Sturm-Liouville operator with Dirichlet boundary conditions. Namely, let $U(x) = \{u_{ij}(x)\}_{i,j=1}^n$ be a C^1-function on $[0,T]$ which takes values in real, symmetric $n \times n$ matrices, and consider

$$\boldsymbol{A} = -D^2 I_n + U(x)$$

where I_n is the $n \times n$ identity matrix. The differential operator $\boldsymbol{A}$ with Dirichlet boundary conditions is self-adjoint on the Hilbert space $L^2([0,T],\mathbb{C}^n)$ of $\mathbb{C}^n$-valued functions, and has a pure point spectrum accumulating to ∞. Its regularized determinant $\det'\boldsymbol{A}$ and characteristic determinant $\det(\boldsymbol{A}-\lambda\boldsymbol{I})$, where I is the identity operator in $L^2([0,T],\mathbb{C}^n)$, are defined as in the $n=1$ case. Let $\boldsymbol{Y}(x,\lambda)$ be the solution of the differential equation

$$-\boldsymbol{Y}'' + U(x)\boldsymbol{Y} = \lambda \boldsymbol{Y}$$

satisfying initial conditions

$$\boldsymbol{Y}(0,\lambda) = 0, \quad \boldsymbol{Y}'(0,\lambda) = I_n$$

and put $\boldsymbol{D}(\lambda) = \det \boldsymbol{Y}(T,\lambda)$. The entire function $\boldsymbol{D}(\lambda)$ has properties similar to that of $d(\lambda)$, and the following analog of Theorem 5.1 holds.

Proposition 5.1. The characteristic determinant $\det(\boldsymbol{A}-\lambda\boldsymbol{I})$ is given by the formula

$$\det(\boldsymbol{A}-\lambda\boldsymbol{I}) = 2^n \boldsymbol{D}(\lambda)$$

Moreover,

$$\frac{\det(\boldsymbol{A}-\lambda\boldsymbol{I})}{\det'\boldsymbol{A}} = (-\lambda)^\delta \prod_{\lambda_n \neq 0} \left(1 - \frac{\lambda}{\lambda_n}\right)$$

where δ is the multiplicity of the eigenvalue $\lambda = 0$.

Problem 5.1 (Gelfand-Levitan trace identity). Prove that

$$\sum_{n=1}^{\infty} \left(\lambda_n - \lambda_n^{(0)} - c\right) = \frac{1}{2T}\int_0^T u(x)dx - \frac{u(0)+u(T)}{4}$$

where $\lambda_n^{(0)} = \left(\frac{\pi n}{T}\right)^2$ and $c = \frac{1}{T}\int_0^T u(x)dx$.

5.2. Periodic boundary conditions. As in the previous section, we assume that $u(x) \in C^1([0,T],\mathbb{R})$. The Sturm-Liouville operator $A = -D^2 + u(x)$ with periodic boundary conditions is self-adjoint on $L^2(0,T)$ with the domain

$$D(A) = \left\{y(x) \in W^{2,2}(0,T) : y(0) = y(T) \text{ and } y'(0) = y'(T)\right\}$$

It has a pure point spectrum with the eigenvalues

$$\lambda_0 < \lambda_1 \leq \lambda_2 < \cdots < \lambda_{2n-1} \leq \lambda_{2n} < \cdots$$

accumulating to ∞. Moreover, as $n \to \infty$,

$$\lambda_{2n-1} = \frac{4\pi^2 n^2}{T^2} + c + O\left(n^{-2}\right), \quad \lambda_{2n} = \frac{4\pi^2 n^2}{T^2} + c + O\left(n^{-2}\right) \tag{5.16}$$

where c is the same as in (5.1). Replacing, if necessary, A by $A - (\lambda_0 + a)\,I$ with $a > 0$, we can always assume that $\lambda_0 > 0$, and define

$$\vartheta_A(t) = \sum_{n=0}^{\infty} e^{-\lambda_n t}, t > 0$$

Using asymptotics (5.16), we get that as $t \to 0$,

$$\vartheta_A(t) = e^{-ct}\vartheta\left(\frac{4\pi t}{T^2}\right)(1+O(t)) = \frac{a_{-\frac{1}{2}}}{\sqrt{t}} + O(\sqrt{t})$$

where $a_{-\frac{1}{2}} = \frac{T}{2\sqrt{\pi}}$ as in (5.4), but $a_0 = 0$. This allows us to define the regularized determinant $\det' A$ and the characteristic determinant $\det(A - \lambda I)$ exactly as in the previous section. Since $a_0 = 0$, we now get as $\mu \to +\infty$

$$\det(A+\mu I) = e^{\sqrt{\mu}T}\left(1 + O\left(\mu^{-\frac{1}{2}}\right)\right) \tag{5.17}$$

(see the end of the proof of Theorem 5.1).

Here we denote [7] by $y_1(x,\lambda)$ and $y_2(x,\lambda)$ solutions of the Sturm-Liouville equation (5.5) satisfying initial conditions $y_1(0,\lambda) = 1, y_1'(0,\lambda) = 0$ and $y_2(0,\lambda) = 0, y_2'(0,\lambda) = 1$. Solutions y_1 and y_2 are linearly independent for all λ and the matrix

$$Y(x,\lambda) = \begin{pmatrix} y_1(x,\lambda) & y_2(x,\lambda) \\ y_1'(x,\lambda) & y_2'(x,\lambda) \end{pmatrix}$$

satisfies the initial condition $Y(0,\lambda) = I_2$, where I_2 is the 2×2 identity matrix, and has the property $\det Y(x,\lambda) = 1$. For fixed x the matrix $Y(x,\lambda)$ is an entire matrix-valued function of λ having the following asymptotics as $\lambda \to \infty$:

$$Y(x,\lambda) = \begin{pmatrix} \cos\sqrt{\lambda}x & \frac{1}{\sqrt{\lambda}}\sin\sqrt{\lambda}x \\ \sqrt{\lambda}\sin\sqrt{\lambda}x & \cos\sqrt{\lambda}x \end{pmatrix}\left(I_2 + O\left(|\lambda|^{-1}e^{|\operatorname{Re}\sqrt{\lambda}|x}\right)\right) \tag{5.18}$$

By definition, the monodromy matrix of the periodic Sturm-Liouville problem is the matrix

$$T(\lambda) = Y(T,\lambda)$$

The monodromy matrix satisfies $\det T(\lambda) = 1$ and is an entire matrix-valued function. The following result is the analog of Theorem 5.1 for the periodic boundary conditions.

Theorem 5.2. One has

$$\det(A-\lambda I) = -\det{}_2\left(T(\lambda) - I_2\right) = y_1(T,\lambda) + y_2'(T,\lambda) - 2$$

where $\det_2$ is the determinant of a 2×2 matrix. Moreover,

$$\frac{\det(A-\lambda I)}{\det' A} = (-\lambda)^\delta \prod_{\lambda_n \neq 0}\left(1 - \frac{\lambda}{\lambda_n}\right)$$

where $\{\lambda_n\}_{n=0}^\infty$ are the eigenvalues of A, and $0 \le \delta \le 2$ is a multiplicity of the eigenvalue $\lambda = 0$.

Proof. The proof follows closely the proof of Theorem 5.1, and we will assume that $A > 0$. First, in exact analogy with (5.9) we obtain that for $\lambda \neq \lambda_n$,

$$\frac{d}{d\lambda}\log\det(A-\lambda I) = -\operatorname{Tr} R_\lambda$$

where $R_\lambda = (A-\lambda I)^{-1}$. To get a closed expression for the integral kernel $R(x,\xi)$ of the operator R_λ, we use the same variation of parameters method as in the previous section, but now for periodic boundary conditions. As a

result, we obtain that the symmetric, continuous kernel $R_\lambda(x,\xi)$ is given for $x \le \xi$ by the formula

[07] There should be no confusion with the notation in the previous section.

$$R_\lambda(x,\xi) = -\left(y_1(x,\lambda), y_2(x,\lambda)\right)\left(T(\lambda)-I_2\right)^{-1}T(\lambda)\begin{pmatrix} y_2(\xi,\lambda) \\ -y_1(\xi,\lambda)\end{pmatrix}$$
$$= -\operatorname{Tr}_2\left\{\left(T(\lambda)-I_2\right)^{-1}T(\lambda)Z(x,\xi;\lambda)\right\},$$

where Tr_2 in the last formula is the matrix trace and

$$Z(x,\xi;\lambda) = \begin{pmatrix} y_1(x,\lambda)y_2(\xi,\lambda) & y_2(x,\lambda)y_2(\xi,\lambda) \\ -y_1(x,\lambda)y_1(\xi,\lambda) & -y_2(x,\lambda)y_1(\xi,\lambda)\end{pmatrix}.$$

As in the proof of Theorem 5.1, we need to compute $\int_0^T Z(x,x;\lambda)dx$. It readily follows from formula (5.11) and the definition of the monodromy matrix that

$$\int_0^T Z(x,x;\lambda)dx = T^{-1}(\lambda)\frac{d}{d\lambda}T(\lambda).$$

Therefore
$\frac{d}{d\lambda}\log\det(A-\lambda I) = \operatorname{Tr}_2\left(\left(T(\lambda)-I_2\right)^{-1}\frac{d}{d\lambda}T(\lambda)\right) = \frac{d}{d\lambda}\log\det_2\left(T(\lambda)-I_2\right)$, and $\det(A-\lambda I) = C\det\left(T(\lambda)-I_2\right)$. To determine the constant C we set $\lambda=-\mu\to+\infty$ and compare asymptotics (5.17) with the asymptotics

$$\det_2\left(T(-\mu)-I_2\right) = 2-\operatorname{Tr}T(-\mu) = 2-2\cosh\sqrt{\mu}T\left(1+O\left(\mu^{-\frac{1}{2}}\right)\right)$$
$$= -e^{\sqrt{\mu}T}\left(1+O\left(\mu^{-\frac{1}{2}}\right)\right)$$

which follows from (5.18). Thus $C=-1$.
Remark. In Section 3.2 of Chapter 6 we will use Theorem 5.2 for calculating Gaussian Wiener integrals over the loop spaces.

In the special case $u(x)=0$, we have

$$y_1(x,\lambda) = \cos\sqrt{\lambda}x \quad \text{and} \quad y_2(x,\lambda) = \frac{\sin\sqrt{\lambda}x}{\sqrt{\lambda}}$$

so that

$$\det\left(-D^2-\lambda I\right) = 2(\cos\sqrt{\lambda}T-1) = -4\sin^2\frac{\sqrt{\lambda}T}{2} \tag{5.19}$$

Setting $\lambda=-\omega^2<0$, for the operator $A_{i\omega}=-D^2+\omega^2$ we get

$$\det A_{i\omega} = 4\sinh^2\frac{\omega T}{2}, \tag{5.20}$$

and also

$$\det' A_0 = -\lim_{\lambda\to 0^-}\frac{\det(A-\lambda I)}{\lambda} = \lim_{\omega\to 0}\frac{\det' A_{i\omega}}{\omega^2} = T^2. \tag{5.21}$$

Remark. Using that the spectrum of $A_{i\omega}$ consists of double eigenvalues $\lambda_n(\omega) = \left(\frac{2\pi n}{T}\right)^2, n=1,2,...$, and of the simple eigenvalue ω^2, we can derive formulas (5.20)-(5.21) directly, as was done in Section 4.2 for Dirichlet boundary conditions. There is also an analog of the heuristic computation in Section 4.2:

$$\frac{\det A_{i\omega}}{\det' A_0} = \omega^2\prod_{n=1}^{\infty}\frac{\lambda_n(\omega)^2}{\lambda_n(0)^2} = \omega^2\prod_{n=1}^{\infty}\left(1+\frac{\omega^2T^2}{4\pi^2n^2}\right)^2 = \frac{4}{T^2}\sinh^2\frac{\omega T}{2}.$$

A similar result holds for the general second order differential operator $A = -D^2 + v(x)D + u(x)$ on the interval $[0, T]$ with periodic boundary conditions. Namely, repeating the proof of Theorem 5.2, we have the following

Theorem 5.3. For the differential operator $A = -D^2 + v(x)D + u(x)$ one has

$$\begin{aligned}\det(A - \lambda I) &= -e^{-\frac{1}{2}\int_0^T v(x)dx} \det{}_2 \left(T(\lambda) - I_2\right) \\ &= e^{-\frac{1}{2}\int_0^T v(x)dx} \left(y_1(T,\lambda) + y_2'(T,\lambda) - 1 - e^{\int_0^T v(x)dx}\right)\end{aligned}$$

where solutions $y_{1,2}(x, \lambda)$ and the monodromy matrix $T(\lambda)$ are defined by the same formulas as for the case $v(x) = 0$.

In particular, the following result will be used in Section 2.2 of Chapter 8.

Corollary 5.4.

$$\det{}' \left(-D^2 + \omega D\right) = \frac{2T}{\omega} \sinh \frac{\omega T}{2}$$

Proof. The proof is an elementary computation, using Theorem 5.3, an explicit form of the solutions $y_{1,2}(x, \lambda)$, and the formula

$$\det{}' \left(-D^2 + \omega D\right) = -\lim_{\lambda \to 0} \frac{\det\left(-D^2 + \omega D - \lambda I\right)}{\lambda}$$

Remark. Since the operator $-D^2 + \omega D$ on $[0, T]$ with periodic boundary conditions has simple eigenvalues $\lambda_n(a) = \left(\frac{2\pi n}{T}\right)^2 + i\omega \left(\frac{2\pi n}{T}\right), n = -\infty, ..., \infty$, we can also repeat the heuristic computation in Section 4.2:

$$\frac{\det'\left(-D^2 + \omega D\right)}{\det'\left(-D^2\right)} = \prod_{n=1}^{\infty} \left(1 + \frac{\omega^2 T^2}{4\pi^2 n^2}\right) = \frac{2}{\omega T} \sinh \frac{\omega T}{2}$$

A similar result holds for the matrix-valued Sturm-Liouville operator with periodic boundary conditions. Namely, let $U(x) = \{u_{ij}(x)\}_{i,j=1}^n$ be a C^1-function on $[0, T]$ which takes values in real, symmetric $n \times n$ matrices, and consider

$$\boldsymbol{A} = -D^2 I_n + U(x)$$

The differential operator $\boldsymbol{A}$ with periodic boundary conditions is self-adjoint on the Hilbert space $L^2\left([0, T], \mathbb{C}^n\right)$ of $\mathbb{C}^n$-valued functions, and has a pure point spectrum accumulating to ∞. Its regularized determinant $\det'\boldsymbol{A}$ and characteristic determinant $\det(\boldsymbol{A} - \lambda \boldsymbol{I})$, where $\boldsymbol{I}$ is the identity operator in $L^2\left([0, T], \mathbb{C}^n\right)$, are defined as in the $n = 1$ case. Let $\boldsymbol{Y}_1(x, \lambda)$ and $\boldsymbol{Y}_2(x, \lambda)$ be the solutions of the differential equation

$$-\boldsymbol{Y}'' + U(x)\boldsymbol{Y} = \lambda \boldsymbol{Y}$$

satisfying, respectively, the initial conditions

$$\boldsymbol{Y}_1(0, \lambda) = I_n, \quad \boldsymbol{Y}_1'(0, \lambda) = 0 \quad \text{and} \quad \boldsymbol{Y}_2(0, \lambda) = 0, \quad \boldsymbol{Y}_2'(0, \lambda) = I_n.$$

The monodromy matrix $\boldsymbol{T}(\lambda)$ is defined as the following $2n \times 2n$ block matrix:

$$\boldsymbol{T}(\lambda) = \begin{pmatrix} \boldsymbol{Y}_1(T, \lambda) & \boldsymbol{Y}_2(T, \lambda) \\ \boldsymbol{Y}_1'(T, \lambda) & \boldsymbol{Y}_2'(T, \lambda) \end{pmatrix}$$

and is a matrix-valued entire function. The analog of Theorem 5.2 is the following statement.

Proposition 5.2. The characteristic determinant is given by the formula

$$\det(\boldsymbol{A}-\lambda\boldsymbol{I})=(-1)^n\det{}_{2n}\left(\boldsymbol{T}(\lambda)-I_{2n}\right)$$

where $\det_{2n}$ is the determinant of a $2n\times 2n$ matrix, and

$$\frac{\det(\boldsymbol{A}-\lambda\boldsymbol{I})}{\det'\boldsymbol{A}}=(-\lambda)^\delta\prod_{\lambda_n\neq 0}\left(1-\frac{\lambda}{\lambda_n}\right)$$

where δ is the multiplicity of the eigenvalue $\lambda=0$.

Problem 5.2. Prove Theorem 5.3.

Problem 5.3. Derive Corollary 5.4.

5.3. First order differential operators. Here we continue to assume that $u(x)\in C^1([0,T],\mathbb{R})$, and consider the first order differential operator

$$A=D+u(x)$$

on the interval $[0,T]$ with periodic boundary conditions $y(0)=y(T)$. The equation

$$y'+u(x)y=\lambda y$$

has an explicit solution $y(x)=Ce^{\lambda x-\int_0^x u(\tau)d\tau}$, which is periodic if and only if $\lambda=\lambda_n$, where

$$\lambda_n=u_0+\frac{2\pi in}{T},\quad n\in\mathbb{Z},\qquad\text{and}\qquad u_0=\frac{1}{T}\int_0^T u(x)dx$$

Thus the spectrum of the operator A coincides with the spectrum of the operator $A_0=D+u_0$.

Proposition 5.3. For $u_0>0$,

$$\det(D+u(x))=1-e^{-u_0T}$$

and $\det' D=T$ for $u_0=0$.

Proof. The zeta-function of the operator A with $u_0>0$ is given by the series

$$\zeta_A(s)=\sum_{n=-\infty}^{\infty}\frac{1}{\lambda_n^s}$$

where $\lambda_n^{-s}=e^{-s\log\lambda_n}$ with the principal branch of the logarithm. This series is absolutely convergent for $\operatorname{Re}s>1$. Introducing the Hurwitz zeta-function

$$\zeta(s,a)=\sum_{n=0}^{\infty}\frac{1}{(n+a)^s}$$

where $\operatorname{Re}a>0$ and $\operatorname{Re}s>1$, we can rewrite $\zeta_A(s)$ as

$$\zeta_A(s)=\left(\frac{2\pi}{T}\right)^{-s}\left(e^{-\frac{\pi is}{2}}\zeta(s,a)+e^{\frac{\pi is}{2}}\zeta(s,\bar a)\right)+\frac{1}{u_0^s},\quad a=1-\frac{u_0T}{2\pi}i$$

It is well known that the Hurwitz zeta-function admits a meromorphic continuation to the whole s-plane with single simple pole at $s=1$ with residue 1 , and

$$\zeta(0,a)=\frac{1}{2}-a,\quad \frac{\partial\zeta}{\partial s}(0,a)=\log\Gamma(a)-\frac{1}{2}\log 2\pi$$

Using the classical formula

$$\Gamma(1+z)\Gamma(1-z)=\frac{\pi z}{\sin\pi z}$$

we obtain

$$\frac{d\zeta_A}{ds}(0) = \log|\Gamma(a)|^2 - \log u_0 T + \frac{u_0 T}{2}$$
$$= -\log\left(e^{\frac{u_0 T}{2}} - e^{-\frac{u_0 T}{2}}\right) + \frac{u_0 T}{2}$$

so that $\det(D + u(x)) = 1 - e^{-u_0 T}$. Finally, $\zeta_D(s) = \lim_{u_0 \to 0}\left(\zeta_A(s) - u_0^{-s}\right)$, and we get

$$\det' D = \lim_{u_0 \to 0} \frac{\det'(D + u_0)}{u_0} = T$$

Remark. For $u_0 < 0$ one should use the branch of the logarithm with the cut along the positive semi-axis, and the above arguments give

$$\det(D + u(x)) = 1 - e^{u_0 T}$$

Remark. One can also consider the operator $A = D + u(x)$ on the interval $[0, T]$ with anti-periodic boundary conditions $y(0) = -y(T)$. The corresponding eigenvalues are

$$\lambda_n = u_0 + \frac{\pi i(2n+1)}{T}, n \in \mathbb{Z}$$

and the passage from periodic to anti-periodic boundary conditions amounts to replacing u_0 by $u_0 + \frac{\pi i}{T}$. It follows from Proposition 5.3 that for $u_0 > 0$,

$$\det(D + u(x)) = 1 + e^{-u_0 T}.$$

Remark. Proposition 5.3 is very useful for calculating Gaussian path integrals in the holomorphic representation, discussed in Section 2.4. As an example, consider the harmonic oscillator with the Wick symbol $H(\bar{a}, a) = \omega\left(\bar{a}a + \frac{1}{2}\hbar\right)$. Formula (2.16) expresses the trace $\operatorname{Tr} e^{-\frac{1}{\hbar}TH}$ as a path integral in the holomorphic representation. On the other hand, using the explicit form of the eigenvalues $E_n = \omega\hbar\left(n + \frac{1}{2}\right)$, we immediately get

$$\operatorname{Tr} e^{-\frac{1}{\hbar}TH} = \sum_{n=0}^{\infty} e^{-\frac{1}{\hbar}E_n T} = \frac{e^{-\frac{1}{2}\omega T}}{1 - e^{-\omega T}} = \frac{1}{2\sinh\frac{\omega T}{2}}$$

Comparing with (2.16), we obtain that

$$\int\!\!\int_{\left\{\begin{array}{l}\bar{a}(0) = \bar{a}(T)\\ a(0) = a(T)\end{array}\right\}} e^{-\frac{1}{\hbar}\int_0^T(\bar{a}\dot{a} + \omega\bar{a}a)dt}\mathscr{D}\bar{a}\mathscr{D}a = \frac{1}{\det(D + \omega)}, \tag{5.22}$$

which should be considered as a special analog of the finite-dimensional Gaussian integration in the complex domain - formula (3.3).

Problem 5.4. Give a direct proof of formula (5.22).

8.1.6 6. Semi-classical asymptotics - II

Here we consider the semi-classical asymptotics - the asymptotics of the propagator [8] $K_\hbar(\boldsymbol{q}', t'; \boldsymbol{q}, t)$ as $\hbar \to 0$. We compare the heuristic method, based on the Feynman path integral representation (1.26), with the rigorous analysis, based on the short-wave asymptotics, derived in Section 6.1 of Chapter 3.

6.1. Using the Feynman path integral. Start with the Lagrangian $L(q, \dot{q}) = \frac{1}{2}m\dot{q}^2 - V(q)$ for a classical particle with one degree of freedom. The propagator $K_\hbar(q', t'; q, t)$ is given by

[08] Here the dependence on the Planck constant $\hbar$ is introduced explicitly.

the Feynman path integral (1.20), and we will formally apply the stationary phase method to investigate its behavior as $\hbar \to 0$. As in Section 4, we assume that there is a unique classical trajectory $q_{\rm cl}(\tau)$ connecting points q and q' at times t and t', set $q(\tau) = q_{\rm cl}(\tau) + y(\tau)$, and consider the expansion (4.1), i.e.,

$$S(q) = S_{\rm cl} + \frac{1}{2}m \int_t^{t'} \left(\dot{y}^2 - u(\tau)y^2\right) d\tau + O\left(y^3\right)$$

where $u(\tau) = \frac{1}{m}V''\left(q_{\rm cl}(\tau)\right)$ and

$$S_{\rm cl} = \int_t^{t'} \left(\frac{1}{2}m\dot{q}_{\rm cl}^2 - V\left(q_{\rm cl}\right)\right) d\tau = S\left(q', t'; q, t\right).$$

According to the stationary phase method (see Section 2.3 in Chapter 2), the leading contribution to the Feynman integral (1.20) as $\hbar \to 0$ comes from a critical point of the action functional - the classical trajectory $q_{\rm cl}(\tau)$. Thus we obtain as $\hbar \to 0$,

$$\begin{aligned} K_\hbar\left(q', t'; q, t\right) &\simeq e^{\frac{i}{\hbar}S_{\rm cl}} \int_{\substack{y(t')=0 \\ y(t)=0}} e^{\frac{im}{2\hbar}\int_t^{t'}\left(\dot{y}^2 - u(\tau)y^2\right)d\tau} \mathscr{D}y \\ &= \sqrt{\frac{m}{\pi i \hbar \det A}} \exp\left\{\frac{i}{\hbar}S\left(q', t'; q, t\right)\right\}. \end{aligned} \tag{6.1}$$

Here A is the corresponding Jacobi operator - a second order differential operator $-D^2 - u(\tau)$ on the interval $[t, t']$ with Dirichlet boundary conditions. (We are assuming that the potential $V(q)$ is sufficiently smooth so that $u(\tau) \in C^1\left([t, t']\right)$.) Formula (6.1) is a remarkably simple expression which shows a deep relation between semi-classical asymptotics of a quantum mechanical propagator and classical motion.

Remark. When $u(\tau) = \frac{1}{m}V''\left(q_{\rm cl}(\tau)\right)$, the regularized determinant of the differential operator $A = -D^2 - u(\tau)$ on the interval $[t, t']$ with Dirichlet boundary conditions can be expressed entirely in terms of the classical trajectory $q_{\rm cl}(\tau)$. Namely, differentiating Newton's equation

$$m\ddot{q} = -V'(q), \tag{6.2}$$

with respect to τ, we find that the function $y(\tau) = \dot{q}_{\rm cl}(\tau)$ satisfies the differential equation $Ay = 0$. When $y(t) = \dot{q}_{\rm cl}(t) = 0$, the function [9]

$$y_1(\tau) = \frac{y(\tau)}{\dot{y}(t)}$$

satisfies initial condition (5.6) (where the interval $[0, T]$ is replaced by the interval $[t, t']$). According to Theorem 5.1, we have in this case,

$$\det A = 2y_1\left(t'\right) = -2m\frac{\dot{q}_{\rm cl}\left(t'\right)}{V'(q)}. \tag{6.3}$$

In order to find the solution $y_1(\tau)$ of the differential equation $Ay = 0$ for the case $y(t) \neq 0$, observe that the Wronskian $\dot{y}_1 y - \dot{y} y_1$ of its two solutions is constant on $[t, t']$. Using (5.6) we get

$$\dot{y}_1 y - \dot{y} y_1 = y(t),$$

[09] Here we assume that $\dot{y}(t) \neq 0$, so that $V'(q) \neq 0$.

and solving this differential equation we obtain

$$y_1(\tau) = y(\tau)y(t)\int_t^\tau \frac{ds}{y^2(s)}.$$

Thus we get the formula

$$\det A = 2y(t)y\left(t'\right)\int_t^{t'} \frac{d\tau}{y^2(\tau)}, \quad y(\tau) = \dot{q}_{\mathrm{cl}}(\tau) \tag{6.4}$$

which expresses the fluctuating factor in the semi-classical asymptotics of the propagator in terms of the classical motion.

Similarly, for the case of n degrees of freedom, when

$$L = \frac{1}{2}m\dot{\boldsymbol{q}}^2 - V(\boldsymbol{q}),$$

and $V(\boldsymbol{q}) \in C^3\left(\mathbb{R}^n, \mathbb{R}\right)$, we obtain

$$K_\hbar\left(\boldsymbol{q}', t'; \boldsymbol{q}, t\right) \simeq \left(\frac{m}{\pi i\hbar}\right)^{\frac{n}{2}} \frac{1}{\sqrt{\det \boldsymbol{A}}} e^{\frac{i}{\hbar}S(\boldsymbol{q}', t'; \boldsymbol{q}, t)} \tag{6.5}$$

as $\hbar \to 0$, where $\boldsymbol{A} = -D^2 - U(\tau)$ and

$$U(\tau) = \frac{\partial^2 V}{\partial \boldsymbol{q}^2}\left(\boldsymbol{q}_{\mathrm{cl}}(\tau)\right) = \left\{\frac{\partial^2 V}{\partial q_i \partial q_j}\left(\boldsymbol{q}_{\mathrm{cl}}(\tau)\right)\right\}_{i,j=1}^n.$$

6.2. Rigorous derivation. Let $K_\hbar\left(q, q', t\right)$ be the fundamental solution of the Schrdinger equation - the solution of the Cauchy problem (1.3) and (1.5). Since $K_\hbar\left(q', t'; q, t\right) = K_\hbar\left(q', q, T\right)$, where $T = t' - t$, we need to find the asymptotics of a fundamental solution $K_\hbar\left(q, q', T\right)$ as $\hbar \to 0$. The solution of this problem can be divided into two parts.

1. Find the short-wave asymptotics - asymptotics as $\hbar \to 0$ of the solution $\psi_\hbar(q, T)$ of the Cauchy problem for the Schrdinger equation

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial q^2} + V(q)\psi$$

with the initial condition

$$\psi_\hbar(q, t)|_{t=0} = \varphi(q)e^{\frac{i}{\hbar}s(q)},$$

where $s(q), \varphi(q) \in C^\infty(\mathbb{R}, \mathbb{R})$, and the amplitude $\varphi(q)$ has compact support.

2. Using the representation

$$\delta\left(q - q_0\right) = \frac{\varphi(q)}{2\pi\hbar}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}\xi(q - q_0)}d\xi$$

where φ has compact support and satisfies $\varphi\left(q_0\right) = 1$, express $K_\hbar\left(Q, q_0, T\right)$ as an integral over $d\xi$ of solutions of the Schrdinger equation with initial amplitude $\varphi(q)$ and initial phase $s(q, \xi) = \xi\left(q - q_0\right)$. Use asymptotics from part 1 to evaluate the resulting integral by the stationary phase method as $\hbar \to 0$.

The problem in the first part was solved in Section 6.1 in Chapter 3, so we proceed to the second part. For fixed ξ, let $\psi_\hbar(q, t; \xi)$ be the solution of the Schrdinger equation with the initial amplitude $\varphi(q)$ and the initial phase $s(q) = \xi\left(q - q_0\right)$. By the superposition principle,

$$K_\hbar(Q,q_0,T)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\psi_\hbar(Q,T;\xi)d\xi \tag{6.6}$$

Let $\gamma(t;q,\xi)$ be the classical trajectory - the solution of Newton's equation (6.2) with the initial conditions

$$\gamma(0;q,\xi)=q \quad \text{and} \quad \dot\gamma(0;q,\xi)=\frac{\xi}{m} \tag{6.7}$$

As in Section 2.3 of Chapter 1, here we assume that the mapping $q\mapsto Q=\gamma(T;q,\xi)$ is a diffeomorphism, and denote by $q=q(\xi,Q)$ the corresponding inverse function,

$$\gamma(T;q(\xi,Q),\xi)=Q \tag{6.8}$$

The asymptotics of $\psi_\hbar(Q,T;\xi)$ as $\hbar\to 0$ is given by formula (6.13) in Section 6.1 of Chapter 3 , where $p(q)=\frac{\partial s}{\partial q}=\xi$, so that the characteristic ending at Q has the initial momentum ξ and the initial coordinate $q=q(\xi,Q)$. Substituting this expression into (6.6), we obtain

$$K_\hbar(Q,q_0;T)\simeq\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\varphi(q(\xi,Q))\left|\frac{\partial\gamma}{\partial q}(T;q(\xi,Q),\xi)\right|^{-\frac12}$$
$$\times\exp\left\{\frac{i}{\hbar}\left(S(Q,q(\xi,Q);T)+\xi\left(q(\xi,Q)-q_0\right)\right)\right\}d\xi$$

To apply the stationary phase method to this integral, we need to find the critical points of the function $S(Q,q(\xi,Q);T)+\xi\left(q(\xi,Q)-q_0\right)$. Using the formula

$$\frac{\partial S}{\partial q}(Q,q;T)=-p=-\xi$$

which follows from Proposition 2.2 in Section 2.3 of Chapter 1, we obtain

$$\frac{\partial}{\partial\xi}\left(S(Q,q(\xi,Q);T)+\xi\left(q(\xi,Q)-q_0\right)\right)$$
$$=-\xi\frac{\partial q}{\partial\xi}(\xi,Q)+q(\xi,Q)-q_0+\xi\frac{\partial q}{\partial\xi}(\xi,Q)=q(\xi,Q)-q_0$$

so that a single critical point ξ_0 is determined from the equation $q\left(\xi_0,Q\right)=q_0$. The prefactor in the stationary phase method is given by

$$\varphi\left(q_0\right)\left|\frac{\partial\gamma}{\partial q}\left(T;q_0,\xi_0\right)\frac{\partial q}{\partial\xi}\left(\xi_0,Q\right)\right|^{-\frac12}$$

which can be simplified using $\varphi\left(q_0\right)=1$ and the equation

$$\frac{\partial\gamma}{\partial\xi}+\frac{\partial\gamma}{\partial q}\frac{\partial q}{\partial\xi}=0$$

which follows from (6.8). Thus the final expression for the semi-classical asymptotics is

$$K_\hbar(Q,q_0;T)\simeq\frac{1}{\sqrt{2\pi i\hbar}}\left|\frac{\partial\gamma}{\partial\xi}\left(T;q_0,\xi_0\right)\right|^{-\frac12}e^{\frac{i}{\hbar}S(Q,q_0;T)} \tag{6.9}$$

It is remarkable that formula (6.9), after the identification $Q=q'$ and $q_0=q$, coincides with formula (6.1)! Indeed, they have exactly the same exponential factors, and equality of the corresponding prefactors follows from the following result.

Lemma 6.1. Let $\gamma(t;q,\xi)$ be the classical trajectory with the initial conditions (6.7). Then

$$\frac{\partial\gamma}{\partial\xi}(T;q,\xi)=\frac{1}{2m}\det A, \tag{6.10}$$

where A is the differential operator $-D^2-u(t)$ on the interval $[0,T]$ with Dirichlet boundary conditions, and $u(t)=\frac{V''(\gamma(t,q,\xi))}{m}$.

Proof. Differentiating equation (6.2) with respect to ξ, we obtain that $y(t)=\frac{\partial\gamma}{\partial\xi}(t;q,\xi)$ satisfies the differential equation

$$m\ddot{y}=-V''(\gamma(t,q,\xi))y,$$

so that $Ay=0$. Differentiating initial conditions (6.7) with respect to ξ, we get

$$y(0)=0 \quad \text{and} \quad \dot{y}=\frac{1}{m},$$

so that by Theorem 5.1, $\det A=2my(T)$.

Remark. One can get another remarkable formula for the prefactor in representation (6.9). Namely, differentiating $\frac{\partial S}{\partial q}(Q,q;T)=-\xi$ with respect to Q we get

$$\frac{\partial^2 S}{\partial q\partial Q}=-\frac{\partial\xi}{\partial Q}$$

where $Q=\gamma(T;q,\xi)$. Thus (6.9) can be rewritten entirely in terms of the classical action

$$K_\hbar\left(Q,q_0;T\right)\simeq\frac{1}{\sqrt{2\pi i\hbar}}\left|\frac{\partial^2 S}{\partial q\partial Q}\left(Q,q_0;T\right)\right|^{\frac{1}{2}}e^{\frac{i}{\hbar}S(Q,q_0;T)} \tag{6.11}$$

Remark. When assumptions in Section 2.3 of Chapter 1 are not satisfied, there are several characteristics connecting points q_0 and Q, and the situation becomes more complicated. In this case we have

$$K_\hbar\left(Q,q_0,T\right)\simeq\sum_j\frac{1}{\sqrt{2\pi i\hbar}}\left|\frac{\partial\gamma}{\partial\xi}\left(T;q_0,\xi_j\right)\right|^{-\frac{1}{2}}e^{\frac{i}{\hbar}S(Q,q_0,\xi_j;T)-\frac{\pi i}{2}\mu_j}$$

where ξ_j is the initial momentum, and μ_j is the Morse index of the characteristic $\gamma\left(t;q_0,\xi_j\right)$ (see Section 6.1 in Chapter 3).

The case of n degrees of freedom is considered similarly. Using shortwave asymptotics (6.14) in Section 6.1 of Chapter 3 , we obtain as $\hbar\to 0$,

$$K_\hbar\left(\boldsymbol{Q},\boldsymbol{q}_0,T\right)\simeq(2\pi i\hbar)^{-\frac{n}{2}}\left|\det\left(\frac{\partial\boldsymbol{Q}}{\partial\boldsymbol{\xi}}\left(\boldsymbol{q}_0,\boldsymbol{\xi}_0\right)\right)\right|^{-\frac{1}{2}}e^{\frac{i}{\hbar}S(\boldsymbol{Q},\boldsymbol{q}_0;T)} \tag{6.12}$$

where $\boldsymbol{Q}=\gamma\left(t,\boldsymbol{q}_0,\boldsymbol{\xi}_0\right)$. Using the equation

$$\frac{\partial\boldsymbol{\xi}}{\partial\boldsymbol{Q}}=-\frac{\partial^2 S}{\partial\boldsymbol{q}\partial\boldsymbol{Q}}=-\left\{\frac{\partial^2 S}{\partial q_i\partial Q_j}\right\}_{i,j=1}^{n}$$

(6.12) can be rewritten as

$$K_\hbar\left(\boldsymbol{Q},\boldsymbol{q}_0;T\right)\simeq(2\pi i\hbar)^{-\frac{n}{2}}\left|\det\left(\frac{\partial^2 S}{\partial\boldsymbol{q}\partial\boldsymbol{Q}}\left(\boldsymbol{Q},\boldsymbol{q}_0;T\right)\right)\right|^{\frac{1}{2}}e^{\frac{i}{\hbar}S(\boldsymbol{Q},\boldsymbol{q}_0;T)}$$

Here $\det\frac{\partial^2 S}{\partial\boldsymbol{q}\partial\boldsymbol{Q}}$ is known as the van Vleck determinant.

Problem 6.1. Justify all computations in this section.

8.1.7 7. Notes and references

The path integral approach to quantum mechanics was developed by Feynman in his 1942 Princeton thesis, and was published in [Fey48]. In addition to the classic text [FH65] - the best introduction to Feynman path integrals in configuration space, written from a physics perspective - we also refer the reader to a modern
textbook [DR01]. The Feynman path integral in the phase space was introduced by Feynman [Fey51] in 1951 and by Tobocman [Tob56] in 1956. Nowadays it is a very useful method in quantum field theory (see, e.g., Faddeev's Les Houches lectures [Fad76] and the monograph [FS91]). Our derivation of the Feynman path integral in Section 1 is standard and follows monograph [RS75], which also contains a complete proof of the Kato-Lie-Trotter formula. As we mentioned in Section 1, this approach establishes only the L^2-convergence of finite-dimensional approximations like (1.15) and (1.23) to the propagator. We refer the reader to the paper [Fuj80] for the proof of the convergence in other topologies on functional spaces, and to the monograph [AHK76] for the rigorous definition of Feynman path integrals as infinite-dimensional Fresnel integrals.

In Section 2 we follow the outline in [Ber71a] and [Fad76, FS91], and rigorously derive formulas (2.1) and (2.6) for the *pq* and *qp*-symbols of the evolution operator by using explicit relations between the symbols and the propagator. However, corresponding formulas (2.9) and (2.13) for the Weyl and Wick symbols of the evolution operator were derived only heuristically. As was already emphasized in [Ber71a], in this case one needs to justify formulas (2.8) and (2.11). This nontrivial problem was only recently solved in [Dyn98] for a large class of symbols, and we refer to this paper for further details and references. However, following [Fad76, FS91], we carefully treat boundary conditions for the Wick symbol, deriving the correct expression (2.14) (as opposed to the formula in [Ber71a]). Material in Section 3 is standard, and in our exposition we made a special emphasis on the details of computation related to the Morse index. The formula for the propagator of the harmonic oscillator in Proposition 3.1 is called the Feynman-Souriau formula in [DR01]. The relation between formula (3.6) for the propagator of the harmonic oscillator and the Mehler identity for Hermite-Tchebyscheff polynomials, was stated in [FH65]. For the answer to Problem 3.2 we refer the reader to [Ber71a] (after correcting the typos), and for the elegant heuristic solution of Problem 3.3 - to [FS91].

Besides having a conceptual meaning, the path integral formalism is a very convenient computational tool, since it allows us to use, albeit at a heuristic level, such methods of finite-dimensional integration as change of variables, integration by parts, and stationary phase approximation. There is a vast literature devoted to the applications of Feynman path integration in quantum physics. We only mention a perturbative expansion of the propagator using Feynman diagrams [FH65], which is nowadays the main computational method in quantum mechanics and quantum field theory (see also lectures [Kaz99] for the rigorous treatment of a finitedimensional example). For more applications see [DR01], and references therein.

The idea of computing Gaussian path integrals by evaluating separately the classical contribution and the fluctuation factor goes back to [FH65], and Problems 4.1 and 4.4 are taken from this source. In Section 4 we emphasized the role of the
zeta-function regularized determinants of differential operators, by considering the simplest example of the operator $A = -D^2$. We refer the reader to the textbook [Apo76] for the basic properties of the Riemann zeta-function. Our proof of Lemma 4.1 can be considered as a simplified one-dimensional analog of the derivation of the first Kronecker limit formula given in [Lan87]. For the case of Laplace operators on compact Riemannian manifolds, the definition (4.5) of a regularized determinant $\det' A$ (under the name analytic torsion) was given in [**RS71**], and the operator zeta-function $\zeta_A(s)$ was introduced in [MP49]. A similar notion of a perturbation determinant goes back to M.G. Krein [Kre62]; according to Problem 2.6 in Section 2.2 of Chapter 3, the transition coefficient $a(\sqrt{\lambda})$ is the perturbation determinant of $H - \lambda I$,

where H is a one-dimensional Schrdinger operator. We also note that regularized determinants of differential operators have been extensively used in quantum field theory. The corresponding definition was given by V.A. Fock in 1937 and J. Schwinger in 1951, and is similar to (4.5). It is currently known [IZ80] as the Fock-Schwinger proper time method.

In general, the proof of meromorphic continuation of the zeta-function $\zeta_A(s)$ of an elliptic operator A, and its regularity at $s = 0$, uses the theory of complex powers A^{-s}, developed in [See67] (or the short-time asymptotics $t \to 0$ of $\operatorname{Tr} e^{-At}$ - the trace of a heat kernel of A - when A is non-negative [Gil95]). In Section 5 we are using an elementary approach to the short-time asymptotics of the heat kernel, which is based on the large n asymptotics of the eigenvalues of the corresponding boundary value Sturm-Liouville problems. The monograph [LS91] contains all the facts used in Sections 5.1 and 5.2. The coefficients $a_{-\frac{1}{2}}$ and a_0 in formula (5.4), and in their analogs for the periodic case, are called Seeley coefficients. Our proof of the key relation (5.13) and its analog for the periodic case uses Wronskian identities (5.11), and goes back to the papers [Fad57, BF60] on the trace identities for onedimensional Schrdinger operators (see also Problem 2.6 in Section 2.2 of Chapter 3). The theorem that "the operator trace is equal to the matrix trace", used in Sections 5.1 and 5.2, as well as the properties of the Fredholm determinant, can be found in the classic monograph [GK69]. Problem 5.1– the Gelfand-Levitan trace identity – is taken from the paper [GL53] (see also [Dik58] for its generalization). Properties of the Hurwitz zeta-function, used in Section 5.3, are proved in [Apo76]. For the general approach to characteristic determinants of the n-th order differential operators on the interval with matrix coefficients and Dirichlet or periodic boundary conditions, we refer to [BFK91, BFK95].

Our exposition in Section 6 follows [GS77], with simplifications arising from considering the case of one degree of freedom. Lemma 6.1 establishes the equivalence between the heuristic approach in Section 6.1 using path integrals, and the rigorous approach in Section 6.2 using short-wave asymptotics. We refer to [GS77] and [MF81] for the details. Also, see [Foc78] for the relation between the van Vleck determinant and canonical transformation in classical mechanics, and [DR01] for the examples.

8.1.8 Path Integral Formalism

вывод интеграла по траекториям

метод происходит в измерениях на каждой поверхности.?????
это эквивалентно вставке полного набора наблюдаемых.
итак, разобьем на N интервалов наш интервал времени

$$\left\langle q_F \left| e^{-iHT} \right| q_I \right\rangle = \left\langle q_F \left| e^{-iH\delta t} e^{-iH\delta t} ... e^{-iH\delta t} \right| q_I \right\rangle$$

Теперь воспользуемся тем фактом, что $|q\rangle$ образует полный набор состояний, то есть $\int dq|q\rangle\langle q| = 1$.

Вставим 1 между всеми этими множителями $e^{-iH\delta T}$ и запишем

$$\begin{gathered}\left\langle q_F \left| e^{-iHT} \right| q_I \right\rangle = \\ = \left(\prod_{j=1}^{N-1} \int dq_j\right) \left\langle q_F \left| e^{-iH\delta t} \right| q_{N-1} \right\rangle \left\langle q_{N-1} \left| e^{-iH\delta t} \right| q_{N-2} \right\rangle ... \\ \cdots \left\langle q_2 \left| e^{-iH\delta t} \right| q_I \right\rangle\end{gathered}$$

$$\begin{gathered}\left\langle q_{j+1} \left| e^{-i\delta t\left(\hat{p}^2/2m\right)} \right| q_j \right\rangle = \int \frac{dp}{2\pi} \left\langle q_{j+1} \left| e^{-i\delta t\left(\hat{p}^2/2m\right)} \right| p \right\rangle \langle p|q_j\rangle = \\ = \int \frac{dp}{2\pi} e^{-i\delta t\left(p^2/2m\right)} \langle q_{j+1}|p\rangle \langle p|q_j\rangle = \\ = \int \frac{dp}{2\pi} e^{-i\delta t\left(p^2/2m\right)} e^{ip(q_{j+1}-q_j)}\end{gathered}$$

Вычисляя интеграл по p, получаем

$$\left\langle q_{j+1}\left|e^{-i\delta t\left(\hat{p}^2/2m\right)}\right|q_j\right\rangle=\left(\tfrac{-i2\pi m}{\delta t}\right)^{1/2}e^{\left[im(q_{j+1}-q_j)^2\right]/2\delta t}=$$
$$=\left(\tfrac{-i2\pi m}{\delta t}\right)^{1/2}e^{i\delta t(m/2)\left[(q_{j+1}-q_j)^2/\delta t\right]^2}$$

Подставляя это выражение в (3), приходим к

$$\left\langle q_F\left|e^{-iHT}\right|q_I\right\rangle=\left(\frac{-i2\pi m}{\delta t}\right)^{N/2}\prod_{j=0}^{N-1}\int dq_j e^{i\delta t(m/2)}\sum_{j=1}^{N-1}\left[\left(q_{j+1}-q_j\right)/\delta t\right]^2$$

с $q_0\equiv q_I$ и $q_N\equiv q_F$

$$\int Dq(t)=\lim_{N\to\infty}\left(\frac{-i2\pi m}{\delta t}\right)^{N/2}\prod_{j=1}^{N-1}\int dq_j$$

Таким образом, мы получили представление в виде интеграла по траекториям

$$\left\langle q_F\left|e^{-iHT}\right|q_I\right\rangle=\int Dq(t)e^{i\int\limits_0^T dt\frac{1}{2}m\dot{q}^2}$$

$$\int dq_F\int dq_I\left\langle F|q_F\right\rangle\left\langle q_F\left|e^{-iHT}\right|q_I\right\rangle\left\langle q_I|I\right\rangle$$

или, если смешать обозначения Шредингера и Дирака, в виде

$$\int dq_F\int dq_I\Psi_F\left(q_F\right)^*\left\langle q_F\left|e^{-iHT}\right|q_I\right\rangle\Psi\left(q_I\right)$$

$$Z=\int Dq(t)e^{-\int\limits_0^T dt\left[\frac{1}{2}m\dot{q}^2+V(q)\right]}$$

связь интеграла по траекториям с измерениями

пока что думаю, на каждом этапе мы измеряем.

наивный подсчет траекторий

вспомним из научпопа эксперимент с двумя щелями и запишем это все количественно.
сперва давайте добавим одну щель.
потом вторую.
суммируется вот так вот

О проблемах с нестрогим подходом

(пока не въехал, в чем проблема делать как мы делали в квантмехе? там что-то говорят про это, потом узнаю еще раз)

О строгом подходе

(по идее из теории меры тут ответ может быть запишу. пока не планирую этим заниматься, потому что не хочу с математиками общаться.)

О схожести интеграла по траекториям в квантмехе и КТП (??)

(подумаю, хз)

8.2 Path Integral Formulation of QM: Advanced Ideas

8.2.1 Typical Path Integral by Kiselev

нерелятивистская частица через интеграл по траекториям

Рассмотрим эволюцию состояния $|\Psi(t')\rangle$, заданного в начальный момент времени t' в координатном представлении

$$|\Psi(t')\rangle = \int |q'\rangle \, \mathrm{d}q' \Psi(q', t'), \quad \Psi(q', t') = \langle q'|\Psi(t')\rangle,$$

где q'-обобщенная координата (для простоты-в одномерном случае). Тогда согласно общему формализму состояние в момент времени t получается в результате действия оператора эволюции $\hat{U}(t, t')$

$$|\Psi(t)\rangle = \hat{U}(t, t') |\Psi(t')\rangle,$$

где

$$\hat{U}(t, t') = \hat{\mathrm{T}} \exp\left\{ -\frac{\mathrm{i}}{\hbar} \int_{t'}^{t} \hat{H} \, \mathrm{d}t \right\}, \quad \hat{U}(t', t') = 1.$$

Здесь оператор эволюции записан в общем виде как символ "Т-экспоненты", т.е. понимается в виде предела произведения бесконечно малых сдвигов по времени, строго упорядоченных в порядке возрастания моментов времени, а нормировка записана с учетом ненулевого значения исходного момента времени.

В соответствии с таким разбиением интервала $t - t'$ на N отрезков, так что $\mathrm{d}t = (t - t')/N$, при $N \to \infty$ бесконечно малый сдвиг по времени $t' \to t_1 = t' + \mathrm{d}t$ дает

$$|\Psi(t' + \mathrm{d}t)\rangle = \int \exp\left\{ -\frac{\mathrm{i}}{\hbar} \hat{H}(\hat{p}, \hat{q}, t_1) \, \mathrm{d}t \right\} |q'\rangle \, \mathrm{d}q' \Psi(q', t') + \mathcal{O}\left(\mathrm{d}t^2\right),$$

и, подставляя единичные операторы в координатном и импульсном представлениях, находим

$$\hat{H}(\hat{p}, \hat{q}, t) = \frac{\hat{p}^2}{2m} + V(\hat{q}, t),$$

очевидно,

$$\langle p|\hat{H}(\hat{p}, \hat{q}, t)|q\rangle = \mathcal{H}(p, q, t)\langle p|q\rangle,$$

где $\mathcal{H}(p, q, t)$ - гамильтониан классической системы. Тогда

$$\begin{aligned}
\left\langle p_1 \left| \exp\left\{ -\frac{\mathrm{i}}{\hbar} \hat{H}(\hat{p}, \hat{q}, t_1) \, \mathrm{d}t \right\} \right| q' \right\rangle &= \left\langle p_1 \left| \left\{ \mathbb{1} - \frac{\mathrm{i}}{\hbar} \hat{H}(\hat{p}, \hat{q}, t_1) \, \mathrm{d}t \right\} \right| q' \right\rangle + \mathcal{O}\left(\mathrm{d}t^2\right) = \\
&= \langle p_1|q'\rangle \left\{ 1 - \frac{\mathrm{i}}{\hbar} \mathcal{H}(p_1, q', t_1) \, \mathrm{d}t \right\} + \mathcal{O}\left(\mathrm{d}t^2\right) = \\
&= \langle p_1|q'\rangle \exp\left\{ -\frac{\mathrm{i}}{\hbar} \mathcal{H}(p_1, q', t_1) \, \mathrm{d}t \right\} + \mathcal{O}\left(\mathrm{d}t^2\right).
\end{aligned}$$

Пренебрегая в этих выражениях членами второго порядка малости по инкременту времени, введем обозначение $q_0 = q'$ и в (13.3) учтем, что

$$\langle q_1|p_1\rangle = \mathrm{e}^{\mathrm{i}p_1 q_1/\hbar}, \quad \langle p_1|q_0\rangle = \mathrm{e}^{-\mathrm{i}p_1 q_0/\hbar},$$

и в простейшем случае, когда гамильтониан есть сумма кинетической и потенциальной энергии, найдем

$$|\Psi\left(t_1\right)\rangle = \int |q_1\rangle \, \frac{\mathrm{d}q_1 \, \mathrm{d}p_1}{2\pi\hbar} \mathrm{e}^{\frac{i}{\hbar}[p_1(q_1-q')-\mathcal{H}(p_1,q_0,t_1)\mathrm{d}t]} \mathrm{d}q' \Psi\left(q', t'\right).$$

В общем случае при переходе от классического гамильтониана к квантовому возникает проблема упорядочивания некоммутирующих между собой наблюдаемых - координаты и импульса - так, чтобы оператор гамильтониана

конечно, приводит к различным квантовым обобщениям классической теории.

анзатц Вейля (????)

Что касается самой процедуры упорядочивания, то укажем стандартную схему - анзатц Вейля. Пусть дана классическая величина как функция импульса и координаты, $F(p,q)$. Вычислим ее фурье-образ

$$\mathcal{F}(u,v) = \int \mathrm{d}p \, \mathrm{d}q \mathrm{e}^{\mathrm{i}(up+vq)} F(q,p)$$

и построим оператор, упорядоченый по Вейлю, как обратный образ с операторами в экспонентах

$$\hat{F}(\hat{p},\hat{q}) = \int \frac{\mathrm{d}u \, \mathrm{d}v}{(2\pi)^2} \mathrm{e}^{-\mathrm{i}(u\hat{p}+v\tilde{q})} \mathcal{F}(u,v).$$

Этот оператор заведомо эрмитов, если исходная величина F вещественна, а значит, $\mathcal{F}^*(u,v) = \mathcal{F}(-u,-v)$, и эрмитово сопряжение оператора $\hat{F}$ после замены переменных интегрирования $u \mapsto -u, v \mapsto -v$ приводит к искомому тождеству $\hat{F} = \hat{F}^\dagger$.

Вычислим, например, оператор, соответствующий упорядочиванию Вейля для величины $F = pq$. Преобразование Фурье для линейной функции

$$\int \mathrm{d}p p \mathrm{e}^{\mathrm{i}up} = \frac{\partial}{\mathrm{i}\partial u} \int \mathrm{d}p \mathrm{e}^{\mathrm{i}up} = 2\pi \frac{\partial}{\mathrm{i}\partial u} \delta(u),$$

дает фурье-образ

$$\mathcal{F}(u,v) = -(2\pi)^2 \delta'(u)\delta'(v).$$

Тогда обратное преобразование приводит к

$$\hat{F}(\hat{p},\hat{q}) = -\int \frac{\mathrm{d}u \, \mathrm{d}v}{(2\pi)^2} \mathrm{e}^{-\mathrm{i}(u\hat{p}+v\hat{q})} (2\pi)^2 \delta'(u)\delta'(v) = -\left. \frac{\partial^2}{\partial u \partial v} \mathrm{e}^{-\mathrm{i}(u\hat{p}+v\hat{q})} \right|_{u=v=0},$$

так что элементарное разложение экспоненты в ряд до членов квадратичных по аргументу

$$\begin{aligned} \mathrm{e}^{-\mathrm{i}(u\hat{p}+v\hat{q})} &= 1 - \mathrm{i}(u\hat{p}+v\hat{q}) - \frac{1}{2}(u\hat{p}+v\hat{q})^2 + \ldots \\ &= 1 - \mathrm{i}(u\hat{p}+v\hat{q}) - \frac{1}{2}\left(u^2\hat{p}^2 + uv\hat{p}\hat{q} + uv\hat{q}\hat{p} + v^2\hat{q}^2\right) + \ldots \end{aligned}$$

приводит к эрмитово самосопряженному оператору

$$\hat{F} = \frac{1}{2}(\hat{p}\hat{q} + \hat{q}\hat{p})$$

Ясно также, что для функций коммутирующих наблюдаемых, например, для функции, зависящей только от импульса или только от координаты, упорядочивание Вейля

сводится к стандартной подстановке в функцию соответствующего оператора (импульса или координаты). В общем случае вычислим матричный элемент

$$H_{10} = \left\langle q_1 | \hat{H}(\hat{p},\hat{q},t) | q_0 \right\rangle = \int \langle q_1|p\rangle \frac{\mathrm{d}p}{2\pi\hbar} \left\langle p | \hat{H}(\hat{p},\hat{q},t) | q_0 \right\rangle$$

в схеме с упорядочиванием по Вейлю. Для этого следует записать гамильтониан в виде

$$\hat{H}(\hat{p},\hat{q},t) = \int \frac{\mathrm{d}u\ \mathrm{d}v}{(2\pi)^2} \mathrm{e}^{-\mathrm{i}(u\hat{p}+v\hat{q})} \mathcal{H}(u,v,t),$$

где $\mathcal{H}(u,v,t)$ - фурье-образ функции Гамильтона в классической механике $\mathcal{H}(p,q,t)$. Следовательно, необходимо найти матричный элемент

$$\left\langle p \left| \mathrm{e}^{-\mathrm{i}(u\tilde{p}+v\tilde{q})} \right| q_0 \right\rangle,$$

который легко вычисляется согласно общей формуле Бейкера-Хаусдорфа для произведения экспонент операторов A и B, коммутирующих с их коммутатором $[A,B]$,

$$\mathrm{e}^{A+B} = \mathrm{e}^{-\frac{1}{2}[A,B]} \mathrm{e}^{A} \mathrm{e}^{B}$$

так что

$$\mathrm{e}^{-\mathrm{i}(u\hat{p}+v\hat{q})} = \mathrm{e}^{-\frac{1}{2}\mathrm{i}^2 uv[\hat{p},\hat{q}]} \mathrm{e}^{-\mathrm{i}u\hat{p}} \mathrm{e}^{-\mathrm{i}v\hat{q}}$$

и в силу $[\hat{p},\hat{q}] = -\mathrm{i}\hbar$ получаем

$$\left\langle p \left| \mathrm{e}^{-\mathrm{i}(u\hat{p}+v\tilde{q})} \right| q_0 \right\rangle = \mathrm{e}^{-\frac{1}{2}\mathrm{i}\hbar uv} \mathrm{e}^{-\mathrm{i}up} \mathrm{e}^{-\mathrm{i}vq_0} \langle p|q_0\rangle.$$

Значит,

$$H_{10} = \int \frac{\mathrm{d}p}{2\pi\hbar} \frac{\mathrm{d}u\ \mathrm{d}v}{(2\pi)^2} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(q_1-q_0-\hbar u)} \mathrm{e}^{-\mathrm{i}vqq_0} \mathrm{e}^{-\frac{1}{2}\mathrm{i}\hbar uv\mathcal{H}(u,v,t).}$$

Однако интегрирование по импульсу дает дельта-функцию для переменной u:

$$\int \frac{\mathrm{d}p}{2\pi\hbar} \mathrm{e}^{\frac{i}{\hbar}p(q_1-q_0-\hbar u)} = \delta\left(q_1 - q_0 - \hbar u\right),$$

а значит, под интегралом в H_{10} можно произвести интегрирование по u, что приводит к следующему преообразованию аргумента в экспоненте

$$v\left(q_0 + \frac{1}{2}\hbar u\right) = v\left(q_0 + \frac{1}{2}\left(q_1 - q_0\right)\right) = \frac{1}{2}v\left(q_1 + q_0\right).$$

Тогда, если ввести срединную точку

$$\bar{q}_1 = \left(q_1 + q_0\right)/2,$$

То

$$\begin{aligned} H_{10} &= \int \mathrm{d}u \delta\left(q_1 - q_0 - \hbar u\right) \int \frac{\mathrm{d}v}{(2\pi)^2} \mathrm{e}^{-\mathrm{i}\varepsilon\bar{q}_1} \mathcal{H}(u,v,t) = \\ &= \int \mathrm{d}u \int \frac{\mathrm{d}p}{2\pi\hbar} \mathrm{e}^{\hbar p(q_1-q_0)-\mathrm{i}up} \int \frac{\mathrm{d}v}{(2\pi)^2} \mathrm{e}^{-\mathrm{i}v\bar{q}_1} \mathcal{H}(u,v,t) = \\ &= \int \frac{\mathrm{d}p}{2\pi\hbar} \mathrm{e}^{\frac{i}{\hbar}p(q_1-q_0)} \int \frac{\mathrm{d}u\ \mathrm{d}v}{(2\pi)^2} \mathrm{e}^{-\mathrm{i}(up+v\bar{q}_1)} \mathcal{H}(u,v,t). \end{aligned}$$

В итоге берется обратное преобразование Фурье для классических величин

$$\int \frac{\mathrm{d}u\ \mathrm{d}v}{(2\pi)^2} \mathrm{e}^{-\mathrm{i}(up+v\bar{q}_1)} \mathcal{H}(u,v,t) = \mathcal{H}\left(p,\bar{q}_1,t\right),$$

и Таким образом, упорядочивание Вейля приводит к тому, что классический гамильтониан берется в срединной точке координаты. В остальном проведенный

ранее вывод матричного элемента гамильтониана в виде суммы кинетической энергии, которая задается импульсом, и потенциала, который задается в точке начального положения частицы (в данном случае это q_0) остается в силе. Итак, бесконечно малый шаг эволюции от начального состояния $|\Psi(t')\rangle$ давал нам при $t_1 = t' + \mathrm{d}t$ в случае, когда гамильтониан - это сумма потенциальной и кинетической энергии, следующее состояние:

$$|\Psi(t_1)\rangle = \int |q_1\rangle \frac{\mathrm{d}q_1\ \mathrm{d}p_1}{2\pi\hbar} \mathrm{e}^{\frac{i}{\hbar}[p_1(q_1-q')-\mathcal{H}(p_1,q_0,t_1)\mathrm{d}t]} \mathrm{d}q' \Psi(q',t'),$$

которое в случае гамильтониана общего вида с упорядочиванием по Вейлю, как мы показали, переходит в

$$|\Psi(t_1)\rangle = \int |q_1\rangle \frac{\mathrm{d}q_1\ \mathrm{d}p_1}{2\pi\hbar} \mathrm{e}^{\frac{i}{\hbar}[p_1(q_1-q_0)-\mathcal{H}(p_1,\bar{q}_1,t_1)\mathrm{d}t]} \mathrm{d}q_0 \Psi(q_0,t'),$$

где $q_0 = q'$, а $\bar{q}_1 = (q_1+q_0)/2$ - срединная точка. Но это же выражение можно записать с помощью оператора эволюции $\hat{U}(t_1,t')$,

$$|\Psi(t_1)\rangle = \int |q_1\rangle \mathrm{d}q_1 \left\langle q_1 \left| \hat{U}(t_1,t_0) \right| q_0 \right\rangle \mathrm{d}q_0 \Psi(q_0,t'),$$

где $t_0 = t'$ - время начального состояния, так что

$$\left\langle q_1 \left| \hat{U}(t_1,t_0) \right| q_0 \right\rangle = \int \frac{\mathrm{d}p_1}{2\pi\hbar} \mathrm{e}^{\frac{i}{\hbar}[p_1(q_1-q_0)-\mathcal{H}(p_1,\bar{q}_1,t_1)\mathrm{d}t]}.$$

Разбиение интервала эволюции на бесконечно малые отрезки длиной $\mathrm{d}t \to 0$ точками $t_k = t_{k-1} + \mathrm{d}t$ при $k = \overline{\{1,N\}}$ и $t_N = t$ позволяет построить конечное состояние в момент времени t как результат последовательного действия операторов эволюции на каждом бесконечно малом шаге,

$$\begin{aligned} |\Psi(t)\rangle = \lim_{N\to\infty} \hat{U}(t_N,t_{N-1}) ... \hat{U}(t_{k-1}+\mathrm{d}t,t_{k-1}) ... \hat{U}(t_1,t_0) |\Psi(t_0)\rangle = \\ = \lim_{N\to\infty} \int |q_n\rangle \mathrm{d}q_N \left\langle q_N \left| \hat{U}(t_N,t_{N-1}) \right| q_{N-1} \right\rangle ... \mathrm{d}q_k \left\langle q_k \left| \hat{U}(t_k,t_{k-1}) \right| q_{k-1} \right\rangle ... \\ ... \mathrm{d}q_1 \left\langle q_1 \left| \hat{U}(t_1,t_0) \right| q_0 \right\rangle \mathrm{d}q_0 \langle q_0 | \Psi(t_0) \rangle . \end{aligned}$$

Введем срединные точки

$$\bar{q}_k = \frac{1}{2}(q_k + q_{k-1}).$$

Тогда матричный элемент $\left\langle q_k \left| \hat{U}(t_k,t_{k-1}) \right| q_{k-1} \right\rangle$ может быть вычислен точно так же, как мы получили раньше (13.11) путем интегрирования по импульсу, Т. е.

$$\left\langle q_k \left| \hat{U}(t_k,t_{k-1}) \right| q_{k-1} \right\rangle = \int \frac{\mathrm{d}p_k}{2\pi\hbar} \mathrm{e}^{\frac{\mathrm{j}}{\hbar}[p_k(q_k-q_{k-1})-\mathcal{H}(p_k,\bar{q}_k,t_k)\mathrm{d}t]}.$$

Повторим описанную процедуру расчета матричного элемента оператора эволюции $\hat{U}(t_k+\mathrm{d}t,t_k)$ на каждом бесконечно малом шаге эволюции, т.е. N раз, что согласно (13.12) и (13.13) приведет нас к выражению

$$|\Psi(t)\rangle = \lim_{N\to\infty} \int |q_N\rangle \prod_{k=1}^{N} \frac{\mathrm{d}q_k\ \mathrm{d}p_k}{2\pi\hbar} \mathrm{e}^{\frac{\hbar}{k}[p_k(q_k-q_{k-1})-\mathcal{H}(p_k,\bar{q}_k,t_k)\mathrm{d}t]} \mathrm{d}q_0 \Psi(q_0,t'),$$

где $q_0 = q'$. Введем скорость

$$\dot{q}\left(t_k\right) = \frac{q_k - q_{k-1}}{\mathrm{d}t}.$$

Под интегралом произведение экспонент можно записать в виде

$$\prod_{k=1}^{N} \mathrm{e}^{\frac{i}{\hbar}\left[p_k \tilde{q}_k \ \mathrm{d}t - \mathcal{H}\left(p_k, \bar{q}_k, t_k\right)\mathrm{d}t\right]} = \exp\left\{\frac{\mathrm{i}}{\hbar}\sum_{k=1}^{N}\left[p_k \dot{q}_k \ \mathrm{d}t - \mathcal{H}\left(p_k, \bar{q}_k, t_k\right)\mathrm{d}t\right]\right\},$$

и в этом выражении мы, во-первых, введем обозначения

$$p\left(t_k\right) = p_k, \quad q\left(t_k\right) = q_k, \quad \dot{q}\left(t_k\right) = \dot{q}_k,$$

во-вторых, заметим, что срединную координату можно записать в виде

$$\bar{q}_k = \frac{1}{2}\left(q_k + q_{k-1}\right) = \frac{1}{2}\left(q\left(t_k\right) + q\left(t_k\right) - \dot{q}\left(t_k\right)\mathrm{d}t\right) = q\left(t_k\right) - \frac{1}{2}\dot{q}\left(t_k\right)\mathrm{d}t = q\left(t_k\right) + \mathcal{O}(\mathrm{d}t),$$

и поэтому в пределе $N \to \infty$ и $\mathrm{d}t \to 0$ выражение (13.16) сводится к

$$\exp\left\{\frac{\mathrm{i}}{\hbar}\int_{t'}^{t}[p(t)\dot{q}(t) - \mathcal{H}(p(t), q(t), t)]\mathrm{d}t\right\} = \exp\left\{\frac{\mathrm{i}}{\hbar}S\left(t', t\right)\right\},$$

где $S\left(t', t\right)$-классическое действие на траектории с граничными условиями для координат $q\left(t'\right) = q' = q_0$ и $q(t) = q_N$. При этом действие рассматривается в фазовом пространстве $\{q(t), p(t)\}$, где точки $\{q_k, p_k\}$ задают положение частицы в момент времени t_k. Тогда множество точек $\{q_k\}$ образует ломаную траекторию, которая показана на рис. 19. Точно так же можно говорить и о траектории в импульсном пространстве $\{p_k\} \to p(t)$. Другое дело, что формально действие зависит от скорости в координатном пространстве: $\dot{q}_k$ входят в интеграл для действия в (13.16), - а для импульсов тоже можно определить скорость изменения импульса $\dot{p}_k = \left(p_k - p_{k-1}\right)/\mathrm{d}t$ при $k = \overline{\{2, N\}}$, но эта скорость не входит в интеграл для действия в явном виде. Это обусловлено, во-первых, тем, что уравнения движения включают в себя только первую производную импульса по времени, а во-вторых, чисто формально

$$\int p(t)\dot{q}(t)\mathrm{d}t = -\int \dot{p}(t)q(t)\mathrm{d}t + \int \mathrm{d}\{p(t)q(t)\}$$

так что можно рассматривать и траектории в импульсном пространстве, но тогда нужно ставить и другую квантовую задачу: вычислять матричный элемент оператора эволюции не в координатном пространстве, а в импульсном: $\left\langle p'' \left| \hat{U}\left(t, t'\right) \right| p' \right\rangle$ В итоге мы получаем выражение для состояния

$$|\Psi(t)\rangle = \lim_{N\to\infty}\int |q_N\rangle \, \mathrm{d}q' \Psi\left(q', t'\right) \prod_{k=1}^{N} \frac{\mathrm{d}q_k \ \mathrm{d}p_k}{2\pi\hbar} \mathrm{e}^{\frac{\lambda}{k}S(t', t)}$$

Рассмотрим матричный элемент $\langle q''|\Psi\left(t''\right)\rangle = \Psi\left(q'', t''\right)$ - волновую функцию состояния в момент времени $t = t''$, (обратите внимание на пределы изменения номера интервала эволюции k)

$$\langle q''|\Psi\left(t''\right)\rangle = \lim_{N\to\infty}\int \langle q''|q_N\rangle \, \mathrm{d}q' \Psi\left(q', t'\right) \frac{\mathrm{d}q_N \ \mathrm{d}p_N}{2\pi\hbar} \prod_{k=1}^{N-1} \frac{\mathrm{d}q_k \ \mathrm{d}p_k}{2\pi\hbar} \mathrm{e}^{\frac{i}{\hbar}S(t', t'')}$$

Но поскольку

$$\int \langle q''|q_N\rangle \, \mathrm{d}q_N = 1$$

итоговый результат -

$$\langle q''|\Psi\left(t''\right)\rangle = \int \mathrm{d}q' \Psi\left(q',t'\right) \lim_{N\to\infty} \int \frac{\mathrm{d}p_N}{2\pi\hbar} \prod_{k=1}^{N-1} \frac{\mathrm{d}q_k \; \mathrm{d}p_k}{2\pi\hbar} \mathrm{e}^{\frac{i}{k}S(t',t'')}.$$

Сравнивая эту формулу с общим выражением

$$\langle q''|\Psi\left(t''\right)\rangle = \int \mathrm{d}q' \Psi\left(q',t'\right) \langle q'' \left|U\left(t'',t'\right)\right| q'\rangle$$

заключаем, что матричный элемент оператора эволюции задается формулой

$$= \lim_{N\to\infty} \int \frac{\mathrm{d}p_N}{2\pi\hbar} \prod_{k=1}^{N-1} \frac{\mathrm{d}q_k \; \mathrm{d}p_k}{2\pi\hbar} \mathrm{e}^{\frac{i}{\hbar}S(t',t'')} = \int \mathcal{D}q\mathcal{D}p \mathrm{e}^{\frac{i}{\hbar}S(t',t'')},$$

где мера интегрирования получается при предельном переходе к континууму

$$\mathcal{D}q\mathcal{D}p = \lim_{N\to\infty} \frac{\mathrm{d}p_N}{2\pi\hbar} \prod_{k=1}^{N-1} \frac{\mathrm{d}q_k \; \mathrm{d}p_k}{2\pi\hbar},$$

и поэтому фейнмановский интеграл по траекториям называют также континуальным интегралом. Подчеркнем, что матричный элемент - это число или числовая функция, т.е. классический объект, и континуальный интеграл построен из чисто классических величин: траекторий и действия на них. При этом траектории движения в координатном пространстве имеют граничные условия

$$q\left(t'\right) = q', \quad q\left(t''\right) = q'',$$

а траектории в импульсном пространстве не имеют каких-либо определенных граничных условий, и это есть следствие квантового рассмотрения: в классической механике траектории в фазовом пространстве имеют определенные граничные условия - начальные и конечные точки на фазовой плоскости, а в квантовой механике в силу соотношения неопределенности координатаимпульс выбор граничной точки координаты означает, что граничная точка по импульсу имеет бесконечно больпую неопределенность, т.е. произвольна. Физический смысл такого представления матричного элемента в виде интеграла по траекториям прост: амплитуда перехода из точки $q\left(t'\right) = q'$ в точку $q\left(t''\right) = q''$ есть суперпозиция амплитуд для всех траекторий из истодной точки 6 конечнуо, так что каждая траектория 6 фазобом пространв фейнмановской формулировке прослеживается явная связь с принципом Гюйгенса в теории волн, а именно, интеграл по траекториям устанавливает квантовый аналог принципа Гюйгенса.

Классическая механика неявно предполагает, что «прямая траектория, удовлетворяющая уравнениям движения, следующим из принципа экстремальности действия с фиксированными конечными точками, с вероятностью, рабной единице, проходит через бсе промежсточные точки экстремальной траектории.

Проиллюстрируем это утверждение на простейшем примере свободной нерелятивистской частицы (потенциал равен нулю, а все экстремальные траектории - прямые линии в декартовых координатах). Согласно принципу экстремума действия в классической механике между точками начала и конца траектории, q' и q'', соответственно, за время от t' до t'' пролегает единственная прямая траектория.

Рассмотрим промежуточный момент времени $\tilde{t} : t' < \tilde{t} < t''$. Классическая траектория в этот момент времени проходит через точку $\tilde{q} = q(\tilde{t})$. Если теперь рассмотреть распространение частицы последовательно за два интервала времени от t' до $\tilde{t}$ с граничными точками q' и $\tilde{q}$ и от $\tilde{t}$ до t'' с граничньми точками $\tilde{q}$ и q'', то для экстремальной траектории действие

$$S\left(q'', t''; q', t'\right) = S\left(q'', t''; \tilde{q}, \tilde{t}\right) + S\left(\tilde{q}, \tilde{t}; q', t'\right),$$

а произведение амплитуд для отрезков траекторий в точности дает амплитуду для исходной экстремальной траектории. При этом действие удовлетворяет уравнениям Гамильтона-Якоби, в которых берутся частные производные по координатам и времени конечных точек. Итак, разбиение классической траектории промежуточной точкой эволюции на этой же траектории приводит к тождественному преобразованию для амплитуды вероятности, которая соответствует этой экстремальной траектории. Это и значит, что в классике фактически считается, что все промежуточные точки траектории безусловно проходятся частицей с вероятностью, равной единице. Однако в самой постановке задачи заложено условие, что известны только начальная и конечная точки эволюции, а промежуточная точка на траектории не регистрируется. Поэтому допустимо рассмотреть построенные нами выше два интервала эволюции, но с промежуточной точкой в момент времени $\tilde{t}$, отличной от координаты на классической экстремальной траектории в этот момент времени, $\tilde{q}' = \tilde{q} + \delta\tilde{q} \neq \tilde{q}$. Мы можем теперь поставить задачу найти две экстремальные траектории для этих граничных точек. Для свободной частицы задача элементарна: траектория - это ломаная линия из двух отрезков, проходящих по заданным конечным точкам. При этом действие для каждого их этих отрезков опять будет удовлетворять уравнениям Гамильтона-Якобби, но их сумма, конечно, будет отличаться от экстремального действия для траектории в целом, Так как действие для ломаной траектории пе совнадает уравнениям Гамильтона-Якоби по конечной точке эволюции сразу следует, что амплитуды вероятности как для классической экстремальной траектории, так и для ломаной траектории, удовлетворяют одному и тому же уравнению Шрёдингера, которое как раз и строилось по этому принципу!

Поэтому в квантовой механике поступают более аккуратно: если наблюдаются только конечные точки на траектории, необходимо рассмотреть вероятность того, что в промежуточных точках частица движется по экстремальной траектории классической механики или имеют место отклонения от этой классической траектории в промежуточных точках эволюции. Эти отклонения - квантовые флуктуации траектории. Для решения задачи - вероятности флуктуаций в квантовой механике вычисляется амплитуда вероятности прохождения частицы через произвольные промежуточные точки траектории между конечными точками в виде суперпозиции амплитуд вероятности для каждой промежуточной траектории, причем амплитуда A_k на k-той траектории определяется действием S_k на этой траектории,

$A_k = \exp\left\{\mathrm{i}S_k/\hbar\right\}$. Сами промежуточные точки возникают при малых шагах эволюции от исходной точки в промежуточные так, что действие на каждой такой квантовой флуктуации траектории удовлетворяет уравнениям Гамильтона-Якоби (уравнения в частных производных по координатам и времени промежуточной точки), и поэтому, как следствие, суперпозиция амплитуд удовлетворяет уравнению Шрёдингера на каждом шаге эволюции от исходной точки к промежуточным и от промежуточных к последующим промежуточным, и наконец, от промежуточных к конечной точке эволюции. Результат суммирования - амплитуда вероятности - может отличаться от единственного вклада, который в сумму дает классическая экстремальная траектория, и тогда говорят, что причина такого отличия - вклад квантовых флуктуаций траекторий.

Квантовая теория опирается на возможность квантовых флуктуаций траектории.

Она утверждает, что вероятность таких флуктуаций описывается количественно, и способна предсказать вероятностные характеристики квантовых флуктуаций. Это означает, что предсказуемы величины для ансамбля идентичных квантовых состояний. Если ансамбля нет, то возможно говорить только о тех характеристиках, вероятность которых в квантовой теории равна нулю, например, атом водорода с вероятностью, равной нулю, может иметь энергию связи, отличную от допустимого спектра энергий атома водорода в квантовой теории. Вообще же, рассмотрение квантовой системы вне ансамбля никак не связано с волновой функцией, и следовательно, всякое понятие о редукции волновой функции для системы вне ансамбля лишено какоголибо физического смысла и обычно вводится математиками для операций с элементами гильбертова пространства вне связи с реальностью.

Последовательная эволюция квантового состояния от t' до t, а затем от t до t'', где $t'' > t > t'$, выражается в операторном тождестве

$$\hat{U}\left(t'', \tilde{t}\right) \hat{U}\left(\tilde{t}, t'\right) = \hat{U}\left(t'', t'\right).$$

Продемонстрируем, что это может быть зашисано и в терминах интегралов по траекториям. Для этого сначала разобьем интервал от $t' = t_0$ до $\tilde{t} = t_N$ с помощью N точек t_k, как мы это уже делали раньше, и запишем матричный элемент оператора эволюции на этом интервале времени в форме (13.20),

$$\left\langle q_N \left| U\left(\tilde{t}, t'\right) \right| q' \right\rangle = \lim_{N\to\infty} \int \mathrm{e}^{\frac{i}{\hbar}\sum\limits_{k=1}^{N}[p_k\dot{q}_k\ \mathrm{d}t - \mathcal{H}(p_k,\bar{q}_k,t_k)\mathrm{d}t]} \frac{\mathrm{d}p_N}{2\pi\hbar} \prod_{k=1}^{N-1} \frac{\mathrm{d}q_k\ \mathrm{d}p_k}{2\pi\hbar} =$$

$$= \lim_{N\to\infty} \int \frac{\mathrm{d}p_N}{2\pi\hbar} \prod_{k=1}^{N-1} \frac{\mathrm{d}q_k\ \mathrm{d}p_k}{2\pi\hbar} \mathrm{e}^{\frac{i}{\hbar}S(t',\bar{t})} = \int \mathcal{D}q\mathcal{D}p \mathrm{e}^{\frac{i}{\hbar}S(t',\bar{t})}, \quad (13.24)$$

где скорость координаты согласно (13.15)

$$\dot{q}_k = \frac{q_k - q_{k-1}}{\mathrm{d}t},$$

а затем разобьем интервал от $\tilde{t} = t_N$ до $t'' = t_{M+N}$ с помощью M точек t_k, начиная нумерацию точек k с $N+1$ и кончая на $N+M$, и запишем матричный элемент оператора эволюции $= \lim_{M\to\infty} \int \frac{\mathrm{d}p_{N+M}}{2\pi\hbar} \prod_{k=N+1}^{N+M-1} \frac{\mathrm{d}q_k\ \mathrm{d}p_k}{2\pi\hbar} \mathrm{e}^{\frac{i}{\hbar}S\left(\tilde{t},t''\right)} = \int \mathcal{D}q\mathcal{D}p \mathrm{e}^{\frac{i}{\hbar}S\left(\tilde{t},t''\right)} \cdot$ (13.25) Но тогда можно взять матричный элемент операторного соотношения (13.23)

$$\left\langle q'' \left| \hat{U}\left(t'', \tilde{t}\right) \hat{U}\left(\tilde{t}, t'\right) \right| q' \right\rangle = \left\langle q'' \left| \hat{U}\left(t'', t'\right) \right| q' \right\rangle,$$

вставив в него единичный оператор в координатном пространстве

$$1 = \int |q_N\rangle\, \mathrm{d}q_N\, \langle q_N|,$$

Так что

$$\left\langle q'' \left| \hat{U}\left(t'', \tilde{t}\right) \hat{U}\left(\tilde{t}, t'\right) \right| q' \right\rangle = \int \left\langle q'' \left| \hat{U}\left(t'', \tilde{t}\right) \right| q_N \right\rangle \mathrm{d}q_N \left\langle q_N \left| \hat{U}\left(\tilde{t}, t'\right) \right| q' \right\rangle =$$

$$= \lim_{M\to\infty} \lim_{N\to\infty} \int \mathrm{e}^{\frac{i}{\hbar}\sum\limits_{k=1}^{N+M}[p_k\dot{q}_k\ \mathrm{d}t - \mathcal{H}(p_k,\bar{q}_k,t_k)\mathrm{d}t]} \frac{\mathrm{d}p_{N+M}}{2\pi\hbar} \prod_{k=1}^{N+M-1} \frac{\mathrm{d}q_k\ \mathrm{d}p_k}{2\pi\hbar} =$$

$$= \lim_{M\to\infty} \lim_{N\to\infty} \int \frac{\mathrm{d}p_{N+M}}{2\pi\hbar} \prod_{k=1}^{N+M-1} \frac{\mathrm{d}q_k\ \mathrm{d}p_k}{2\pi\hbar} \mathrm{e}^{\frac{i}{\hbar}S(t',t'')} =$$

$$= \int \mathcal{D}q\mathscr{D}p \mathrm{e}^{\frac{i}{\hbar}S(t',t'')} = \left\langle q'' \left| \hat{U}\left(t'', t'\right) \right| q' \right\rangle.$$

Таким образом, мы убедились, что операторная запись (13.23) согласуется с представлением для матричных элементов в формализме интегралов по траекториям (13.27).

Оператор эволюции можно представить как

$$\hat{U}\left(t'',t'\right)=\int \mathrm{d}q''\left|q''\right\rangle \left\langle q''\left|\hat{U}\left(t'',t'\right)\right|q'\right\rangle \mathrm{d}q'\left\langle q'\right|,$$

откуда

$$\hat{U}\left(t'',t'\right)=\int \mathrm{d}q''\mathrm{d}q'\left|q''\right\rangle \left\langle q'\right|\int \mathcal{D}q\mathcal{D}p\mathrm{e}^{\frac{i}{\hbar}S(t',t'')}.$$

Функция Грина через оператор эволюции по Киселеву (??)

Обычно вводят запаздывающую функцию Грина уравнения Шрёдингера

$$\mathrm{i}\hbar\mathcal{G}\left(q'',t'';q',t'\right)\overset{\text{def}}{=}\vartheta\left(t''-t'\right)\left\langle q''\left|U\left(t'',t'\right)\right|q'\right\rangle,$$

где $\vartheta(\cdot)$ - ступенчатая тэта-функция Хевисайда. Если вычислить производную по времени конечной точки эволюции

$$\mathrm{i}\hbar\frac{\partial}{\partial t''}\left\{\vartheta\left(t''-t'\right)\left\langle q''\left|U\left(t'',t'\right)\right|q'\right\rangle\right\}$$

и использовать уравнение Шрёдингера для оператора эволюции в координатном представлении $\left|q''\right\rangle$

$$\mathrm{i}\hbar\frac{\partial}{\partial t''}\left\langle q''\left|U\left(t'',t'\right)\right|q'\right\rangle=\hat{H}\left(q'',\hat{p}'',t''\right)\left\langle q''\left|U\left(t'',t'\right)\right|q'\right\rangle$$

с начальными данными $\left\langle q''\left|U\left(t',t'\right)\right|q'\right\rangle=\left\langle q''\right|\mathbb{1}\left|q'\right\rangle=\delta\left(q''-q'\right)$, а также равенством

$$\mathrm{i}\hbar\frac{\partial}{\partial t''}\vartheta\left(t''-t'\right)=\mathrm{i}\hbar\delta\left(t''-t'\right),$$

То

$$\begin{aligned}&\mathrm{i}\hbar\frac{\partial}{\partial t''}\left\{\mathrm{i}\hbar\mathcal{G}\left(q'',t'';q',t'\right)\right\}=\mathrm{i}\hbar\frac{\partial}{\partial t''}\left\{\vartheta\left(t''-t'\right)\left\langle q''\left|U\left(t'',t'\right)\right|q'\right\rangle\right\}=\\&=\mathrm{i}\hbar\delta\left(t''-t'\right)\left\langle q''\left|U\left(t'',t'\right)\right|q'\right\rangle+\vartheta\left(t''-t'\right)\hat{H}\left(q'',\hat{p}'',t''\right)\left\langle q''\left|U\left(t'',t'\right)\right|q'\right\rangle=\\&=\mathrm{i}\hbar\delta\left(t''-t'\right)\left\langle q''\left|U\left(t',t'\right)\right|q'\right\rangle+\hat{H}\left(q'',\hat{p}'',t''\right)\left\{\vartheta\left(t''-t'\right)\left\langle q''\left|U\left(t'',t'\right)\right|q'\right\rangle\right\}=\\&=\mathrm{i}\hbar\delta\left(t''-t'\right)\delta\left(q''-q'\right)+\hat{H}\left(q'',\hat{p}'',t''\right)\mathrm{i}\hbar\mathcal{G}\left(q'',t'';q',t'\right).\end{aligned}$$

Таким образом, функция Грина (13.29) удовлетворяет уравнению

$$\left\{\mathrm{i}\hbar\frac{\partial}{\partial t''}-\hat{H}\left(q'',p'',t''\right)\right\}\mathcal{G}\left(q'',t'';q',t'\right)=\delta\left(t''-t'\right)\delta\left(q''-q'\right),$$

которое представляет собой уравнение Шрёдингера с дельтаобразньм источником. Решение этого уравнения - отклик на воздействие источника как раз и называют функцией Грина. В терминах функции Грина эволюция состояния вперед во времени дается соотношением

$$\Psi\left(q'',t''\right)=-\frac{\mathrm{i}}{\hbar}\int\mathcal{G}\left(q'',t'';q',t'\right)\Psi\left(q',t'\right)\mathrm{d}q',\quad t''>t'.$$

В простейших случаях, например, для свободной частицы, можно решить это уравнение в явном виде. Однако в этом разделе мы исследуем метод континуального интеграла,

оставляя изложение аппарата запаздывающей функции Грина до рассмотрения теории рассеяния. К действию замкнутой системы $S\left(t',t''\right)$ можно добавить вклад, обусловленный воздействием на систему зависящих от времени внешних сил, которые также называют внешними источниками $j(t)$. Например,

$$S\left(t',t''\right)\mapsto S\left(t',t''\right)+S_{\text{ext}}\left[j\right],\quad S_{\text{ext}}\left[j\right]=\int\limits_{t'}^{t''}\mathrm{d}tq(t)j(t)\equiv q_{(t)}j_{(t)},$$

где в последнем равенстве мы для краткости записи интегралов, в особенности, кратных, ввели правило интегрирования по непрерывным немым индексам [1], которые, чтобы не путать их с тензорными индексами, мы указываем в скобках (в данном случае, по переменной t), в полной аналогии с суммированием по дискретным немым индексам.

Включение внешних сил позволяет более глубоко исследовать свойства физической системы, меняя величину воздействия внешних сил.

Если внешних сил нет, то говорят, что внешние источники j равны нулю, и обычно вводят обозначение для матричного элемента оператора эволюции

$$Z[0]=\left\langle q''\left|U\left(t'',t'\right)\right|q'\right\rangle\big|_{j=0}=\left.\int\mathcal{D}q\mathcal{D}p\mathrm{e}^{\frac{i}{\hbar}S(t',t'')}\right|_{j=0}$$

Классический предел.

При $\hbar\to 0$ под интегралом стоит функция с быстро осциллирующей фазой $S/\hbar$, за исключением случая, когда у действия имеется стационарная точка:

$$\delta S=0,\quad \delta q\left(t'\right)=\delta q\left(t''\right)=0,$$

т.е. вариация действия на траектории с фиксированными концами обращается в нуль. Но это есть не что иное, как принцип наименьшего действия в классической механике. Значит,

$$Z[0]=\int\mathcal{D}q\mathcal{D}p\mathrm{e}^{\frac{1}{\hbar}S(t',t'')}\approx A\mathrm{e}^{\frac{1}{\hbar}S_0(t',t'')}+\text{ квантовые поправки},$$

где S_0 - действие на «прямой классической траектории. Фактически такое доминирование имеет место только тогда, когда точность измерений наблюдаемых в системе существенно уступает точности, с которой можно зарегистрировать вклады от квантовых флуктуаций, и тогда говорят, что квантовые флуктуации очень малы. Ясно, что предел $h\to 0$ подразумевает сравнение величины измеряемого действия S_0 и точности его определения наблюдении квантовых эффектов не имеет смысла.

Интегрирование по импульсу

В случае, когда импульс входит в гамильтониан только квадратично, и в частности, только в кинетическую энергию, интегралы по импульсам в выражении для матричного элемента оператора эволюции в (13.20) можно взять, так как

$$\mathcal{I}_k=\int\limits_{-\infty}^{+\infty}\frac{\mathrm{d}p_k}{2\pi\hbar}\exp\left\{\frac{\mathrm{i}}{\hbar}\left[p_k\dot{q}_k-\frac{p_k^2}{2m}\right]\mathrm{d}t\right\}=\int\limits_{-\infty}^{+\infty}\frac{\mathrm{d}p_k}{2\pi\hbar}\exp\left\{\frac{\mathrm{i}}{\hbar}\left[-\frac{\left(p_k-m\dot{q}_k\right)^2}{2m}+\frac{m\dot{q}_k^2}{2}\right]\mathrm{d}t\right\},$$

откуда

$$\mathcal{I}_k=\mathcal{N}_k\exp\left\{\frac{\mathrm{i}}{\hbar}\frac{m\dot{q}_k^2}{2}\,\mathrm{d}t\right\}$$

где нормировочная константа $\mathcal{N}_p$ не зависит от траектории. Это значит, что в интеграле по траекториям (13.20) после интегррования по импульсам остается только интеграл по координатам, но при этом действие уже зависит не от координат и импульсов, как и должно быть в гамильтоновой механике, а от координат и скоростей, как это имеет место в лагранжевой механике. Тогда

$$Z[0] = \mathcal{N} \int \mathcal{D}q \mathrm{e}^{\frac{1}{\hbar} S(t',t'')},$$

где уже действие зависит только от траектории в координатном пространстве:

$$S\left(t', t''\right) = \int\limits_{t'}^{t''} \mathrm{d}t \left\{ \frac{m\dot{q}^2(t)}{2} - V[q(t), t] \right\},$$

а

$$\mathcal{N} = \lim_{N\to\infty} \prod_{k=1}^{N} \mathcal{N}_k$$

Поворот Вика

При интегрировании для оценки константы $\mathcal{N}_p$ часто используют поворот Вика контура интегрирования по времени. Формально полагают, что

$$\mathrm{d}t = -\mathrm{i}\mathrm{d}t_E,$$

где t_E - вевклидово время (см. рис. 20). Для правомерности такого поворота Рис. 20. Поворот Вика (слева: жирная прямая со стрелками указывает движение в положительном направлении $\mathrm{d}t > 0$ по переменной t вдоль вещественной оси, спрана: жирная прямая со стрелками указывает движение в положительном направлении $\mathrm{d}t_E > 0$ по переменной t_E, что отвечает чисто мнимым значениям $\mathrm{d}t = -\mathrm{i}\mathrm{d}t_E$ и означает поворот жирной прямой со стрелками - вещественной оси в плоскости комплексной переменной t - на угол $-\frac{\pi}{2}$, а образом этой прямой становится ось чисто мнимых значений с обратным следованием точек на оси). необходимо, чтобы на пути смещения контура не было особых точек. Обычно полагают, что это условие выполнено. Тогда при $\mathrm{d}t_E > 0$ стандартный гауссов

интеграл легко берется,

$$\mathcal{N}_k = \int\limits_{-\infty}^{+\infty} \frac{\mathrm{d}p_k}{2\pi\hbar} \exp\left\{ -\frac{1}{\hbar} \frac{\left(p_k - m\dot{q}_k\right)^2}{2m} \, \mathrm{d}t_E \right\} = \sqrt{\frac{m}{2\pi\hbar t_E}}.$$

Отсюда видно, что, во-первых, нормировочный фактор действительно не зависит от параметров траектории и его можно вынести из-под знака континуального интеграла. Во-вторых, в пределе бесконечно малого шага эволюции $\mathrm{d}t_E \to 0$. Поэтому возникает вопрос: как такое сингулярное поведение номировочных констант по времени скажется на значении континуального интеграла в целом? Для корректного определение континуального интеграла необходимо считать $\mathrm{d}t_E$ конечным на всех промежуточных стадиях расчетов и переходить к пределу $\mathrm{d}t_E \to 0$ только в самом конце, когда рассматривают наблюдаемые величины: такая процедура называется «регуляризацией». В качестве примера расчетов с регуляризацией мы предлагаем читателям самостоятельно провести расчет континуального интеграла для свободной нерелятивистской частицы.

Задача 7.1. В формализме интеграла по траекториям, используя определение (13.21), вычислить матричный элемент оператора эволюции для свободной частицы $\langle q''\left|U\left(t'',t'\right)\right|q'\rangle = \int \mathcal{D}q\mathcal{D}p\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S\left(t',q',t'',q''\right)} = \sqrt{\frac{-\mathrm{i}m}{2\pi\hbar(t''-t')}}\exp\left\{\frac{\mathrm{i}}{\hbar}\frac{m}{2}\frac{(q''-q')^2}{t''-t'}\right\}$, проводя интегрирование сначала по координатам, а затем по импульсам с использованием поворота Вика. Обратите внимание, что фазой экспоненты является действие для свободной частицы между заданными граничными точками!

Убедитесь, что при $t = t'' \neq t'$ амплитуда квантового перехода свободной частицы из точки q' в точку $q = q''$, те. $A(t,q) = \langle q\left|U\left(t,t'\right)\right|q'\rangle$ удовлетворяет уравнению Шрёдингера

$$\mathrm{i}\,\hbar\frac{\partial A(t,q)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 A(t,q)}{\partial q^2}.$$

13.2. Т-пРоизведение. Прямая задача исследования отклика квантовой системы на внешнее воздействие - это вычисление матричных элементов для операторов, которые описывают такое воздействие. Для начала рассмотрим матричный элемент упорядоченных по ходу эволюции операторов в картине Шрёдингера,

$$\langle F(\tilde{t})\rangle = \left\langle q''\left|\hat{U}\left(t'',\tilde{t}\right)\hat{F}(\hat{p},\hat{q},\tilde{t})\hat{U}\left(\tilde{t},t'\right)\right|q'\right\rangle, \quad \text{при } t''>\tilde{t}>t'.$$

Физический смысл этого матричного элемента следующий: состояние, которое задается собственным значением координаты q', эволюционирует от момента t' до времени $\tilde{t}$, где на квантовое состояние воздействует оператор $\hat{F}$, и затем система эволюционирует от $\tilde{t}$ до момента времени t'', а насс интересует амплитуда вероятности того, что при $t = t''$ состемä окажется в квантовом состоянии с собственным значением координаты q''. Вставляя операторные единицы в координатном представлении

$$\mathbb{1} = \int |q_N\rangle\,\mathrm{d}q_N\left\langle q_N\right|, \quad \mathbb{1} = \int\left|q_{N+1}\right\rangle\mathrm{d}q_{N+1}\left\langle q_{N+1}\right|,$$

перепипем (13.36) в виде

$$\langle F(\tilde{t})\rangle = \int\left\langle q''\left|\hat{U}\left(t'',\tilde{t}\right)\right|q_{N+1}\right\rangle\mathrm{d}q_{N+1}\left\langle q_{N+1}|\hat{F}(\hat{p},\hat{q},\tilde{t})|q_N\right\rangle\mathrm{d}q_N\left\langle q_N\left|\hat{U}\left(\tilde{t},t'\right)\right|q'\right\rangle.$$

В этом выражении, как мы показали ранее на стр. 234 при выводе матричного элемента гамильтониана (13.8), матричный элемент оператора при квантовании по Вейлю

$$\left\langle q_{N+1}|\hat{F}(\hat{p},\hat{q},\hat{t})|q_N\right\rangle = \int\frac{\mathrm{d}p_{N+1}}{2\pi\hbar}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}p_{N+1}(q_{N+1}-q_N)}\mathcal{F}\left(p_{N+1},\bar{q}_{N+1},\tilde{t}\right),$$

где $\bar{q}_{N+1} = \left(q_{N+1}+q_N\right)/2$ - срединная точка, а $\mathcal{F}\left(p_{N+1},\bar{q}_{N+1},\tilde{t}\right)$ - классическое выражение для величины $\mathcal{F}$ в терминах переменных фазового пространства. Разбивая интервалы эволюции на бесконечно малые шаги так же, как мы это уже делали при выводе произведения операторов эволюции на последовательных промежутках времени (см. стр. 241), найдем

$$\left\langle q_N\left|U\left(\tilde{t},t'\right)\right|q'\right\rangle = \lim_{N\to\infty}\int\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\sum\limits_{k=1}^{N}\left[p_k\dot{q}_k\ \mathrm{d}t-\mathcal{H}(p_k,\bar{q}_k,t_k)\mathrm{d}t\right]}\frac{\mathrm{d}p_N}{2\pi\hbar}\prod_{k=1}^{N-1}\frac{\mathrm{d}q_k\ \mathrm{d}p_k}{2\pi\hbar} =$$

$$= \lim_{N\to\infty}\int\frac{\mathrm{d}p_N}{2\pi\hbar}\prod_{k=1}^{N-1}\frac{\mathrm{d}q_k\ \mathrm{d}p_k}{2\pi\hbar}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t',\bar{t})} = \int\mathcal{D}q\mathcal{D}p\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t',t)},$$

где $\tilde{t} = t_N, t' = t_0$, и

$$\left\langle q_{N+M} \left| U\left(t'', \tilde{t}\right) \right| q_{N+1} \right\rangle = \lim_{M\to\infty} \int \mathrm{e}^{\frac{i}{k}\sum\limits_{k=N+2}^{N+M}[p_k\dot{q}_k\ \mathrm{d}t - \mathcal{H}(p_k,\bar{q}_k,t_k)\mathrm{d}t]} \frac{\mathrm{d}p_{N+M}}{2\pi\hbar} \times \prod_{k=N+2}^{N+M-1} \frac{\mathrm{d}q_k\ \mathrm{d}p_k}{2\pi\hbar} =$$

$$= \lim_{M\to\infty} \int \frac{\mathrm{d}p_{N+M}}{2\pi\hbar} \prod_{k=N+2}^{N+M-1} \frac{\mathrm{d}q_k\ \mathrm{d}p_k}{2\pi\hbar} \mathrm{e}^{\frac{i}{\hbar}S(\bar{t},t'')} =$$

$$= \int \mathcal{D}q\mathcal{D}p \mathrm{e}^{\dot{\hbar}S(E_t,t'')},$$

где $\tilde{t} + \mathrm{d}t = t_{N+1}, t'' = t_{N+M}$. Собирая выражения для матричных элементов, найдем

$$\left\langle q'' \left| \hat{U}\left(t'', \tilde{t}\right) \hat{F}(\hat{p},\hat{q},\tilde{t}) \hat{U}\left(\tilde{t}, t'\right) \right| q' \right\rangle = \times \lim_{M\to\infty} \lim_{N\to\infty} \int \mathrm{e}^{\frac{i}{\hbar}\sum\limits_{k=N+2}^{N+M}[p_k\tilde{q}_k\ \mathrm{d}t - \mathcal{H}(p_k,\bar{q}_k,t_k)\mathrm{d}t]} \frac{\mathrm{d}p_{N+M}}{2\pi\hbar} \prod_{k=N+2}^{N+M-1} \frac{\mathrm{d}q_k\ \mathrm{d}p_k}{2\pi\hbar} \times$$

$$\times \frac{\mathrm{d}q_{N+1}\ \mathrm{d}p_{N+1}}{2\pi\hbar} \mathrm{e}^{\hbar p_{N+1}(q_{N+1}-q_N)} \mathcal{F}\left(p_{N+1}, \bar{q}N+1, t_N\right) \times$$

$$\times e^{\frac{1}{\hbar}} \sum_{k=1}^{N} \left[p_k\dot{q}_k\ \mathrm{d}t - \mathcal{H}\left(p_k,\bar{q}_k,t_k\right)\mathrm{d}t\right] \frac{\mathrm{d}q_N\ \mathrm{d}p_N}{2\pi\hbar} \prod_{k=1}^{N-1} \frac{\mathrm{d}q_k\ \mathrm{d}p_k}{2\pi\hbar}.$$

Если теперь обратить внимание на вклад

$$\mathrm{e}^{\frac{i}{\pi}p_{N+1}(q_{N+1}-q_N)} \mathcal{F}\left(p_{N+1}, \bar{q}_{N+1}, t_N\right)$$

и переписать его с помощью производной по времени

$$q_{N+1} - q_N = \dot{q}_{N+1}\ \mathrm{d}t,$$

То

$$\mathrm{e}^{\frac{1}{\hbar}p_{N+1}\dot{q}N+1\ \mathrm{d}t} \mathcal{F}\left(p_{N+1}, \bar{q}_{N+1}, t_N\right) = \mathrm{e}^{\frac{i}{\hbar}p_{N+1}\dot{q}_{N+1}\ \mathrm{d}t - \frac{1}{\hbar}\mathcal{H}(p_{N+1},\bar{q}_{N+1},t_{N+1})\mathrm{d}t} \tilde{\mathcal{F}}\left(p_{N+1}, \bar{q}_{N+1}, t_{N+1}\right),$$

где величина в пределе бесконечно малого шага эволюции стремиться к классической величине, заданной в момент времени $\tilde{t}$,

$$\lim_{\mathrm{d}t\to 0} \tilde{\mathcal{F}}\left(p_{N+1}, \bar{q}_{N+1}, t_{N+1}\right) = \mathcal{F}(p(\tilde{t}), q(\tilde{t}), \tilde{t}),$$

поскольку

$$p_{N+1} = p\left(t_{N+1}\right) = p(\tilde{t}),$$

$$\bar{q}_{N+1} = q\left(t_{N+1}\right) - \frac{1}{2}\dot{q}\left(t_{N+1}\right)\mathrm{d}t = q\left(t_{N+1}\right) + \mathcal{O}(\mathrm{d}t) = q(\tilde{t}) + \mathcal{O}(\mathrm{d}t),$$

а

$$\mathrm{e}^{-\frac{\hbar}{\hbar}\mathcal{H}(p_{N+1},\bar{q}_{N+1},t_{N+1})dt} = \mathrm{e}^{-\hbar\mathcal{H}(p(\bar{t}),q(\bar{t}),\bar{t})dt} + \mathcal{O}\left(\mathrm{d}t^2\right).$$

Это значит, что предел в (13.37) приводит к стандартному выражению для интеграла по траекториям (обратите внимание на континуальную меру интегрирования и интегральные суммы в показателях экспонент) при $t'' > \tilde{t} > t'$

$$\langle F(\tilde{t})\rangle = \left\langle q'' \left| \hat{U}\left(t'', \tilde{t}\right) \hat{F}(\hat{p},\hat{q},\tilde{t}) \hat{U}\left(\tilde{t}, t'\right) \right| q' \right\rangle =$$

$$= \int \mathcal{D}q\mathcal{D}p \mathrm{e}^{\frac{1}{\hbar}S(t',t'')} \mathcal{F}(p(\tilde{t}), q(\tilde{t}), \tilde{t})$$

Если теперь заметить, что функционал с внешним источником $j_F(t)$ для величины $\mathcal{F}$

$$\mathrm{e}^{\frac{i}{\hbar}S_{\mathrm{ext}}\,[jF]} = \exp\left\{\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t j_F(t)\mathcal{F}(p(t),q(t),t)\right\}$$

при вычислении вариационной производной дает

$$-\,\mathrm{i}\hbar\frac{\delta}{\delta j_F(\bar{t})}\mathrm{e}^{\frac{j}{\hbar}S_{\mathrm{uxt}}[j_F]}\Big|_{jF=0} = \mathcal{F}(p(\tilde{t}),q(\tilde{t}),\tilde{t}),$$

то приходим к формуле

$$\begin{aligned}\langle F(\tilde{t})\rangle &= \int \mathcal{D}q\mathcal{D}p\mathrm{e}^{\frac{i}{\hbar}S(t',t'')}\mathcal{F}(p(\tilde{t}),q(\tilde{t}),\tilde{t}) = \\ &= -\,\mathrm{i}\hbar\frac{\delta}{\delta j_F(\bar{t})}\int \mathcal{D}q\mathcal{D}p\mathrm{e}^{\hbar S(t',t'')+\hbar S_{\mathrm{ext}}[j_F]}\Big|_{jF=0}.\end{aligned}$$

Итак, мы установили, что матричный элемент оператора величины $\hat{F}$ в обкладках оператора эволюции сводится к вычислению интеграла по траекториям со вставкой значения этой величины на траектории в определенный момент времени (13.38), и этот интеграл по траекториям можно найти как вариационную производную от интеграла по траекториям с учетом вклада в действие члена с источником (13.39).

Связь с представлением Гейзенберга (???)

Покажем теперь, как матричный элемент величины $\hat{F}$ в обкладках оператора эволюции связан с матричным элементом этого оператора в представлении Гейзенберга,

$$\hat{F}_H = \hat{U}^{\dagger}\left(t'',t'\right)\hat{F}\hat{U}\left(t'',t'\right).$$

При $t''>\tilde{t}>t'$ $\hat{U}\left(t'',\tilde{t}\right)\hat{F}(\hat{p},\hat{q},\tilde{t})\hat{U}\left(\tilde{t},t'\right) = \hat{U}\left(t'',\tilde{t}\right)\hat{U}\left(\tilde{t},t'\right)\hat{U}^{\dagger}\left(\tilde{t},t'\right)\hat{F}(\hat{p},\hat{q},\tilde{t})\hat{U}\left(\tilde{t},t'\right) =$

$$= \hat{U}\left(t'',\tilde{t}\right)\hat{U}\left(\tilde{t},t'\right)\hat{F}_H(\hat{p},\hat{q},\hat{t}) = \hat{U}\left(t'',t'\right)\hat{F}_H(\hat{p},\hat{q},\tilde{t}),$$

где мы воспользовались определением оператора эволюции, согласно которому $\hat{U}\left(t'',\tilde{t}\right)\hat{U}\left(\tilde{t},t'\right) = \hat{U}\left(t'',t'\right)$. Поэтому матричный элемент

$$\langle F(\tilde{t})\rangle = \left\langle q''\left|\hat{U}\left(t'',\tilde{t}\right)\hat{F}(\hat{p},\hat{q},\tilde{t})\hat{U}\left(\tilde{t},t'\right)\right|q'\right\rangle = \left\langle q''\left|\hat{U}\left(t'',t'\right)\hat{F}_H(\hat{p},\hat{q},\tilde{t})\right|q'\right\rangle$$

можно переписать, если ввести обозначение для начального состояния в момент времени t'

$$|q'\rangle = |\mathrm{in}'\rangle,$$

а для конечного в момент времени t''

$$|q''\rangle = |\text{ out }''\rangle,$$

так что обратная эволюция дает

$$\ddot{U}^{\dagger}\left(t'',t'\right)|q''\rangle = |\mathrm{in}''\rangle.$$

Отсюда

$$\langle F(\tilde{t})\rangle = \left\langle q''\left|\hat{U}\left(t'',t'\right)\hat{F}_H(\hat{p},\hat{q},\tilde{t})\right|q'\right\rangle = \left\langle \mathrm{in}''\left|\hat{F}_H(\hat{p},\hat{q},\tilde{t})\right|\mathrm{in}'\right\rangle,$$

а стало быть, имеет место следующая связь континуального интеграла и матричного элемента оператора в представлении Гейзенберга по in-состояниям

$$\langle F(\tilde{t})\rangle = \left\langle \mathrm{in}'' \left| \hat{F}_H(\hat{p},\hat{q},\bar{t}) \right| \mathrm{in}' \right\rangle = \int \mathcal{D}q\mathcal{D}p \mathrm{e}^{\frac{i}{\hbar}S(t',t'')} \mathcal{F}(p(\hat{t}),q(\tilde{t}),\bar{t})$$
$$= -\mathrm{i}\hbar \frac{\delta}{\delta j_F(\bar{t})} \int \mathcal{D}q\mathcal{D}p \mathrm{e}^{\hbar} S\left(t',t''\right) + \hbar S_{\mathrm{ext}}\ [j_F]\big|_{jF=0}$$

что в конце формулы мы также записали одноточечный коррелятор $\langle F(\tilde{t})\rangle$ через вариационную производную интеграла по траекториям при наличии внешнего источника j_F для оператора $\hat{F}$ согласно (13.39).

Рассмотрим теперь связь интеграла по траекториям от двух физических наблюдаемых с операторным представлением этих величин. Если задан континуальный интеграл от двух величин F и G в моменты времени $t'' > t_1 > t_2 > t'$ $\langle F\left(t_1\right) G\left(t_2\right)\rangle = \int \mathcal{D}q\mathcal{D}p \mathrm{e}^{\frac{i}{\hbar}S(t',t'')} \mathcal{F}\left(p\left(t_1\right),q\left(t_1\right),t_1\right) \mathcal{G}\left(p\left(t_2\right),q\left(t_2\right),t_2\right)$, (13.42) который называют двухточечным коррелятором, то, как мы показали выше три рассмотрении одного оператора в обкладках оператора эволюции на стр. 247, его можно представить как

$$\langle F\left(t_1\right) G\left(t_2\right)\rangle = \left\langle q'' \left| \hat{U}\left(t'',t_1\right) \hat{F} \hat{U}\left(t_1,t_2\right) \hat{G} \hat{U}\left(t_2,t'\right) \right| q' \right\rangle .$$

В этом выражении порядок операторов строго задан условием $t_1 > t_2$! Введем операторы в представлении Гейзенберга, так что

$$\hat{G}_H\left(t_2\right) = \hat{U}^{\dagger}\left(t_2,t'\right) \hat{G} \hat{U}\left(t_2,t'\right)$$

и воспользуемся, во-первых, унитарностью оператора эволюции и, во-вторых, его основным свойством сдвига квантового состояния по времени, например,

$$\hat{U}\left(t_1,t_2\right) \hat{U}\left(t_2,t'\right) = \hat{U}\left(t_1,t'\right).$$

Тогда

$$\hat{U}\left(t'',t_1\right) \hat{F} \hat{U}\left(t_1,t_2\right) \hat{G} \hat{U}\left(t_2,t'\right) = \hat{U}\left(t'',t_1\right) \hat{F} \left\{ \hat{U}\left(t_1,t_2\right) U\left(t_2,t'\right) \right\} \times$$
$$\times \left\{ \hat{U}^{\dagger}\left(t_2,t'\right) \hat{G} \hat{U}\left(t_2,t'\right) \right\} = \hat{U}\left(t'',t_1\right) \hat{F} \hat{U}\left(t_1,t'\right) \hat{G}_H\left(t_2\right) =$$
$$= \left\{ \hat{U}\left(t'',t_1\right) \hat{U}\left(t_1,t'\right) \right\} \hat{F}_H\left(t_1\right) \hat{G}_H\left(t_2\right) = \hat{U}\left(t'',t'\right) \hat{F}_H\left(t_1\right) \hat{G}_H\left(t_2\right).$$

В итоге при $t_1 > t_2$

$$\int \mathcal{D}q\mathcal{D}p \mathrm{e}^{\frac{i}{\hbar}S(t',t'')} \mathcal{F}\left(p\left(t_1\right),q\left(t_1\right),t_1\right) \mathcal{G}\left(p\left(t_2\right),q\left(t_2\right),t_2\right) =$$
$$= \left\langle q'' \left| \hat{U}\left(t'',t'\right) \hat{F}_H\left(t_1\right) \hat{G}_H\left(t_2\right) \right| q' \right\rangle$$

Поэтому после перехода к in-состояниям получаем матричный элемент операторов в представлении Гейзенберга по базису в начальный момент времени при строгом упорядочении операторов по времени $\langle F\left(t_1\right) G\left(t_2\right)\rangle = \int \mathcal{D}q\mathcal{D}p \mathrm{e}^{\frac{i}{\hbar}S(t',t'')} \mathcal{F}\left(p\left(t_1\right),q\left(t_1\right),t_1\right) \mathcal{G}\left(p\left(t_2\right),q\left(t_2\right),t_2\right) = = \langle \mathrm{in} \left| \hat{F}_H\left(t_1\right) \hat{G}_H\left(t_2\right) \right| \mathrm{in}\ '\rangle$. (13.44) Как мы уже знаем, такой оператор хронологического упорядочивания обозначается символом $\hat{\mathrm{T}}$, так что при произвольных значениях моментов времени континуальный интеграл $\langle F\left(t_1\right) G\left(t_2\right)\rangle$ равен матричному элементу T-произведения операторов

$$\left\langle \mathrm{in}'' \left| \hat{\mathrm{T}} \left\{ \hat{F}_H\left(t_1\right) \hat{G}_H\left(t_2\right) \right\} \right| \mathrm{in}' \right\rangle = \begin{cases} \left\langle \mathrm{in}'' \left| \hat{F}_H\left(t_1\right) \hat{G}_H\left(t_2\right) \right| \mathrm{in}\ ' \right\rangle, & t_1 > t_2, \\ \left\langle \mathrm{in}'' \left| \hat{G}_H\left(t_2\right) \hat{F}_H\left(t_1\right) \right| \mathrm{in}\ ' \right\rangle, & t_2 > t_1 \end{cases}$$

Введение внешних источников для операторов за счет добавки к действию вкладов

$$\mathrm{e}^{\frac{i}{\hbar}S_{\mathrm{ext}}\,[j_F]}=\mathrm{e}^{\frac{j}{\hbar}\int dtj_F(t)\mathcal{F}(p(t),q(t),t)},\quad \mathrm{e}^{\frac{\dot{b}}{\hbar}S'_{\mathrm{axt}}\,[j_G]}=\mathrm{e}^{\frac{1}{\hbar}\int \mathrm{d}tj_G(t)\mathcal{G}(p(t),q(t),t)},$$

позволяет получить связь операторного выражения для матричного элемента с интегралом по траекториям, для которого вычисляются вариационные производные, так что двухточечный коррелятор $\langle F\left(t_1\right)G\left(t_2\right)\rangle$ равен

$$\left\langle \mathrm{in}''\left|\hat{\mathrm{T}}\left\{\hat{F}_H\left(t_1\right)\hat{G}_H\left(t_2\right)\right\}\right|\mathrm{in}'\right\rangle=(-\mathrm{i}\hbar)^2\frac{\delta^2}{\delta j_F\left(t_1\right)\delta j_G\left(t_2\right)}Z\left[j_F,j_G\right]\Big|_{jF=jG=0},$$

$$Z\left[j_F,j_G\right]=\int\mathcal{D}q\mathcal{D}p\mathrm{e}^{\frac{i}{\hbar}S(t',t'')+\frac{i}{\hbar}(S_{\mathrm{ext}}\,[jF]+S'_{\mathrm{ext}}\,[jG])}.$$

Обобщение на случай нескольких операторов очевидно. Нас же в квантовой теории будут интересовать, как говорят, T-упорядоченные корреляторы в случае, когда в качестве начального и конечного состояний выступает вакуум, $|\ \mathrm{in}\ '\rangle=|\ \mathrm{in}\ ''\rangle=|\ \mathrm{vac}\ \rangle$. При этом вакуум $|\mathrm{vac}\rangle$ мы трактуем как фоковское состояние $|0\rangle$ для асимптотически свободных элементарных осцилляторов. Тогда, например, для осциллятора вычисляется двухточечный коррелятор обобщенной координаты

$$\begin{aligned}\langle q\left(t_1\right)q\left(t_2\right)\rangle=\mathcal{D}_{(12)}=\mathcal{D}\left(t_1,t_2\right)=\left\langle 0\left|\hat{\mathrm{T}}\left\{\hat{q}\left(t_1\right)\hat{q}\left(t_2\right)\right\}\right|0\right\rangle=\\=(-\mathrm{i}\hbar)^2\frac{\delta^2}{\delta j\left(t_1\right)\delta j\left(t_2\right)}\int\mathcal{D}q\mathcal{D}p\mathrm{e}^{\hbar}S\left(t',t''\right)+\hbar S_{\mathrm{ext}}[j]\big|_{j=0}=\\=\int\mathcal{D}q\mathcal{D}p\mathrm{e}^{\frac{i}{\hbar}S(t',t'')}q\left(t_1\right)q\left(t_2\right),\end{aligned}$$

где мы опустили знак, который указывает на то, что операторы берутся в представлении Гейзенберга, а для действия с внешним источником $j(t)$ ввели стандартное выражение

$$S_{\mathrm{ext}}\,[j]=j_{(t)}q_{(t)}$$

и использовали соглашение об интегрировании по немой переменной t, записанной в виде индекса в скобках.

Поэтому в следующем разделе мы рассмотрим формулировку для оператора эволюции гармонического осциллятора для вакуум-вакуумных переходов, стартуя с более общего построения для когерентных состояний, частнъм случаем которых является вакуум.

Итак, нас интересует следующая постановка задачи: квантовая система находится в начальном вакуумном состоянии, когда на неё начинают действовать внешние силы (источники). Это приводит к тому, что в квантовой системе под воздействием внешних источников происходят виртуальные процессы. В конечном состоянии нас интересует ситуация, когда квантовая система возвращается в состояние вакуума, но виртуальные квантовые процессы приводят к тому, что возникает обратный отклик квантовой системы на конфигурацию внешних источников, т.е. сама квантовая система воздействует на внешние источники. По тому, какой это отклик при разных воздействиях, мы сможем получить полное описание всей квантовой системы по характеристикам внешних источников в начальном и конечном состоянии. Именно, необходимо вычислить амплитуды вероятности перехода от состояния с одними характеристиками внешних источников в начале эволюции к состоянию с те ми же или со всеми другими характеристикам внешних источников в конце эволюции. Такая постановка квантовой задачи - это швингеровский подход к квантовой механике. Если все амплитуды вероятности перехода «вакуумвакуум» вычислены при любых

конфигурациях внешних источников, то задача решена точно. При этом ясно, что вычисление матричных элементов, в которых, например, в начальном состоянии есть кванты, а не вакуум, типа

$$\left\langle 0 \left| \hat{F}\left(t_1\right) \right| 1 \right\rangle$$

сводится к расчету амплитуды перехода «вакуум-вакуум», если воспользоваться операторами рождения квантов в момент начала эволюции $t = t'$,

$$|1\rangle = \hat{a}^{\dagger}\left(t'\right)|0\rangle.$$

Значит,

$$\left\langle 0 \left| \hat{F}\left(t_1\right) \right| 1 \right\rangle = \left\langle 0 \left| \hat{\mathrm{T}}\left\{ \hat{F}\left(t_1\right) \hat{a}^{\dagger}\left(t'\right) \right\} \right| 0 \right\rangle,$$

и задача опять сводится к вычислению вариационных производных амплитуды вероятности перехода «вакуум-вакуум» при наличии соответствующих источников. Более того, поскольку оператор уничтожения квантов при действии на вакуум дает нуль, $\hat{a}\left(t'\right)|0\rangle = 0$, можно записать, что

$$\left\langle 0 \left| \hat{F}\left(t_1\right) \right| 1 \right\rangle = \left\langle 0 \left| \hat{\mathrm{T}}\left\{ \hat{F}\left(t_1\right) \left(\hat{a}^{\dagger}\left(t'\right) + \hat{a}\left(t'\right) \right) \right\} \right| 0 \right\rangle.$$

а так как координата выражается через операторы рождения и уничтожения, как

$$\hat{q}\left(t'\right) = \sqrt{\frac{\hbar}{2m\omega_0}} \left(\hat{a}^{\dagger}\left(t'\right) + \hat{a}\left(t'\right) \right),$$

ТО

$$\left\langle 0 \left| \hat{F}\left(t_1\right) \right| 1 \right\rangle = \sqrt{\frac{2m\omega_0}{\hbar}} \cdot \left\langle 0 \left| \hat{\mathrm{T}}\left\{ \hat{F}\left(t_1\right) \hat{q}\left(t'\right) \right\} \right| 0 \right\rangle.$$

Следовательно, амплитуда вероятности перехода «вакуум-вакуум при наличии внешних источников содержит в себе исчерпывающую информацию о всевозможных многоточечных матричных элементах операторов по различным начальным и конечным состояниям!

Как мы увидим, вычисление амплитуды вероятности перехода «вакуумвакуум означает, что уравнения для амплитуды вероятности - уравнения Швингера-Дайсона в вариационных производных решены. Как можно предположить, число точно решаемых таким способом задач невелико, а природа преподносит нам варианты реальности - квантовые системы, найти точные решения для которых нелегко. В таком случае приходится более детально рассматривать те виртуальные процессы, которые происходят в вакууме при воздействии внешних источников, выделяя среди этих процессов наиболее физически значимые. Для этой ситуации важнейшую роль играет техника диаграмм Фейнмана.

Диаграммы возникают согласно следующему рассмотрению. Вычислим в операторном подходе двухточечный коррелятор в переходах «вакуум-вакуум для осциллятора с частотой ω_0

$$\left\langle q\left(t_1\right) q\left(t_2\right) \right\rangle = \mathcal{D}_{(12)} = \left\langle 0 \left| \hat{\mathrm{T}}\left\{ \hat{q}\left(t_1\right) \hat{q}\left(t_2\right) \right\} \right| 0 \right\rangle.$$

Если гейзенберговские операторы координат записать в терминах операторов рождения и уничтожения

$$\hat{q}(t) = \sqrt{\frac{\hbar}{2m\omega_0}} \left(\hat{a}^{\dagger} \mathrm{e}^{\mathrm{i}\omega_0 t} + \hat{a} \mathrm{e}^{-\mathrm{i}\omega_0 t} \right),$$

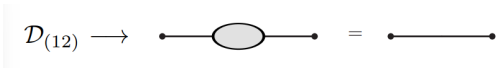
то при $t_1 > t_2$

$$\left\langle 0 \left| \hat{\mathrm{T}} \left\{ \hat{q}\left(t_1\right) \hat{q}\left(t_2\right) \right\} \right| 0 \right\rangle = \frac{\hbar}{2m\omega_0} \left\langle 0 \left| \left(\hat{a}^\dagger \mathrm{e}^{\mathrm{i}\omega_0 t_1} + \hat{a}\mathrm{e}^{-\mathrm{i}\omega_0 t_1} \right) \left(\hat{a}^\dagger \mathrm{e}^{\mathrm{i}\omega_0 t_2} + \hat{a}\mathrm{e}^{-\mathrm{i}\omega_0 t_2} \right) \right| 0 \right\rangle =$$
$$= \frac{\hbar}{2m\omega_0} \left\langle 0 \left| \left(\hat{a}^\dagger \mathrm{e}^{\mathrm{i}\omega_0 t_1} + \hat{a}\mathrm{e}^{-\mathrm{i}\omega_0 t_1} \right) \mathrm{e}^{\mathrm{i}\omega_0 t_2} \right| 1 \right\rangle = \frac{\hbar}{2m\omega_0} \mathrm{e}^{-\mathrm{i}\omega_0 (t_1 - t_2)} \langle 0|\hat{a}|1\rangle =$$
$$= \frac{\hbar}{2m\omega_0} \mathrm{e}^{-\mathrm{i}\omega_0 (t_1 - t_2)}.$$

Эти преобразования состояний имеют вполне ясный физический смысл: сначала при $t_2 < t_1$ из вакуума произопло рождения кванта энергии (частицы с квантом энергии $\hbar\omega_0$, а затем этот квант был уничтожен в момент времени $t_1 > t_2$ и система осталась в вакуумном состоянии. В случае $t_1 < t_2$ операторы координат при раскрытии Т-произведения меняются местами, и вычисления повторяются, но, как легко заметить, оба случая сводятся друг к другу, если в конечном выражении в экспоненте просто поставить положительную разность времен, т.е.

$$\left\langle q\left(t_1\right) q\left(t_2\right) \right\rangle = \mathcal{D}_{(12)} = \left\langle 0 \left| \hat{\mathrm{T}} \left\{ \hat{q}\left(t_1\right) \hat{q}\left(t_2\right) \right\} \right| 0 \right\rangle = \frac{\hbar}{2m\omega_0} \mathrm{e}^{-\mathrm{i}\omega_0 |t_1 - t_2|}.$$

Итак, пропагатор $\mathcal{D}_{(12)}$ описывает рождение кванта из вакуума в момент времени до того, как он исчез в последующий момент времени, так что двухточечному коррелятору, т.е. функции $\mathcal{D}_{(12)}$, имеет смысл сопоставить диаграмму распространения кванта из точки 1 в точку 2



где точки отвечают моментам времени, где рождается и уничтожается квант, а линия - распространение кванта между точками. При этом левая диаграмма обозначает общий случай, когда у осциллятора есть ангармонические взаимодействия, правая - свободный осциллятор. Равенство говорит о том, что для свободного осциллятора пропагатор сводится к простому распространению. Что произойдет при появлении дополнительных взаимодействий, мы рассмотрим позже. Важно, что диаграммы Фейнмана взаимнооднозначно соответствуют многоточечным корреляторам.

релятивистская частица через интеграл по траекториям

осциллятор через интеграл по траекториям

(это же в разделе про осциллятор)

8.2.2 Source and Generating Functional

(тут мы пишем большие формулы, лучше отложить чтение этого раздела, не так это актуально понимать)

Теория

Рассмотрим теперь частицу, на которую действует внешняя сила $j(t)$, зависящая от времени, так что

$$\mathcal{H} = \frac{p^2}{2m} + V(q) - j(t)q$$

В этом случае говорят о гамильтониане с источником j, и ставится задача вычисления амплитуды квантовых переходов при произвольном источнике. В присутствии источника интеграл по траекториям функционально зависит ОТ j

$$Z[j] = \mathcal{N} \int \mathcal{D}q \exp\left\{ \frac{\mathrm{i}}{\hbar} \int\limits_{t'}^{t''} \mathrm{d}t \left[\frac{m\dot{q}^2(t)}{2} - V(q(t)) + j(t)q(t) \right] \right\},$$

Или

$$Z[j] = \mathcal{N} \int \mathcal{D}q \exp\left\{ \frac{i}{\hbar} S\left(t', t'', j\right) \right\}$$

Функциональная замена переменных

$$q(t) \to \tilde{q}(t) = q(t) + \delta q(t), \quad \delta q\left(t'\right) = \delta q\left(t''\right) = 0$$

представляет собой сдвиг, который не изменяет ни меры интегрирования

$$\mathcal{D}q = \mathcal{D}\tilde{q}$$

ни значения функционального интеграла

$$Z[j] = \mathcal{N} \int \mathcal{D}\tilde{q} \exp\left\{ \frac{\mathrm{i}}{\hbar} \tilde{S}\left(t', t'', j\right) \right\}$$

Вычитая из функционала 14.5 самого себя в записи 14.3, находим при $\delta q(t) \to 0$

$$\frac{\delta Z[j]}{\delta q(t)} = 0 \quad \Leftrightarrow \quad \int \mathcal{D}q \frac{\mathrm{i}}{\hbar} \frac{\delta S}{\delta q(t)} \mathrm{e}^{\frac{\mathrm{i}}{\hbar} S(t', t'', j)} = 0.$$

Сюда нужно подставить вариацию Эйлера

$$\frac{\delta S}{\delta q(t)} = -m\ddot{q}(t) - V'(q(t)) + j(t)$$

где V' - производная потенциала по координате, так что

$$\int \mathcal{D}q \left\{ m\ddot{q}(t) + V'(q(t)) - j(t) \right\} \mathrm{e}^{\frac{\mathrm{i}}{\hbar} S(t', t'', j)} = 0.$$

Значит, мы установили квантовый аналог уравнения Лагранжа-Эйлера: уравнения движения остаются справедливыми в смысле интеграла по траекториям.

Наличие источника позволяет преобразовать квантовые уравнения Эйлера-Лагранжа. Действительно,

$$-\mathrm{i}\hbar \frac{\delta Z[j]}{\delta j(t)} = \mathcal{N} \int \mathcal{D}q \cdot q(t) \mathrm{e}^{\frac{\mathrm{i}}{\hbar} S(t', t'', j)}$$

поэтому (14.7) представимо в виде

$$m \frac{\mathrm{d}^2}{\mathrm{d}t^2} \left\{ -\mathrm{i}\hbar \frac{\delta Z[j]}{\delta j(t)} \right\} = -V' \left(-\mathrm{i}\hbar \frac{\delta}{\delta j(t)} \right) Z[j] + j(t) Z[j]$$

Принято делать подстановку

$$Z[j] = \mathcal{N} \mathrm{e}^{\frac{\mathrm{i}}{\hbar} G[j]}$$

тогда

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\left\{\frac{\delta G[j]}{\delta j(t)}\right\} = -\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}G[j]}V'\left(-\mathrm{i}\hbar\frac{\delta}{\delta j(t)}\right)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}G[j]} + j(t)$$

Уравнения в функциональных производных 14.9 и 14.11 суть уравнения Швингера-Дайсона.

Для иллюстрации приведем пример гармонического осциллятора:

$$V(q) \mapsto V_0(q) = \frac{m\omega_0^2}{2}q^2 \Rightarrow V_0'(q) = m\omega_0^2 q$$

откуда уравнение на $G[j]$ для осциллятора принимает вид

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\left\{\frac{\delta G[j]}{\delta j(t)}\right\} = -m\omega_0^2\frac{\delta G[j]}{\delta j(t)} + j(t).$$

Это - функциональное уравнение с источником. В нем можно брать многократные вариационные производные по току в разные моменты времени и потом полагать затем значение тока равным нулю: таким образом возникает бесконечная цепочка уравнений для n-кратных производных функционала $G[j]$ при нулевых значениях внешнего источника! Например, если положить $j = 0$ непосредственно в уравнении 14.12, то получится

$$m\left\{\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \omega_0^2\right\}\mathcal{G}^{(1)}(t) = 0, \quad \mathcal{G}^{(1)}(t) \stackrel{\text{def}}{=} \left.\frac{\delta G[j]}{\delta j(t)}\right|_{j=0}$$

а это значит, что функция $\mathcal{G}^{(1)}(t)$ - это решение уравнения для осциллятора с заданными граничными условиями: $\mathcal{G}^{(1)}(t') = q'$ и $\mathcal{G}^{(1)}(t'') = q''$.

Функционал $G[j]$ можно разложить в функциональный ряд Тейлора

$$G[j] = \mathcal{G}_0 + \int \mathcal{G}^{(1)}(t)j(t)\mathrm{d}t + \\ + \frac{1}{2!}\int \mathcal{G}_{(12)}(t_1,t_2)\,j(t_1)\,j(t_2)\,\mathrm{d}t_1\,\mathrm{d}t_2 + \ldots = \sum_{n=0}^{\infty}\mathcal{G}_{(1\ldots n)}\frac{1}{n!}j_{(1)}\cdots j_{(n)}.$$

Очевидно

$$\mathcal{G}_0 = -\mathrm{i}\hbar\ln\frac{Z[0]}{\mathcal{N}}$$

так что обычно переходят к амплитуде, которая имеет

$$Z[0] = 1$$

чтобы не загромождать формулы, и обозначают её тем же символом, и тогда $\mathcal{G}_0 = 0$

Вариационная производная основного уравнения дает

$$m\frac{\mathrm{d}^2}{\mathrm{d}t_1^2}\left\{\frac{\delta^2 G[j]}{\delta j(t_1)\,\delta j(t_2)}\right\} + m\omega_0^2\frac{\delta^2 G[j]}{\delta j(t_1)\,\delta j(t_2)} = \delta(t_1 - t_2)$$

так что, полагая $j = 0$, находим

$$m\frac{\mathrm{d}^2}{\mathrm{d}t_1^2}\mathcal{G}_{(12)}(t_1,t_2) + m\omega_0^2\mathcal{G}_{(12)}(t_1,t_2) = \delta(t_1 - t_2)$$

т. е. уравнение для двухточечной функции Грина. Домножая это уравнение на $j(t_2)$ и интегрируя по t_2, очевидно, находим уравнение движения для осциллятора с внешней силой (источником)

$$m\left\{\frac{\mathrm{d}^2}{\mathrm{d}t_1^2}+\omega_0^2\right\}\int \mathcal{G}_{(12)}\left(t_1,t_2\right)j\left(t_2\right)\mathrm{d}t_2=j\left(t_1\right)$$

и решение этого уравнения записано в виде вынужденных колебаний

$$q(j;t)=\int \mathcal{G}^{(2)}\left(t,t_2\right)j\left(t_2\right)\mathrm{d}t_2,\quad \mathcal{G}^{(2)}\left(t,t_2\right)=\mathcal{G}_{(t2)},$$

причем общее решение получается суммированием свободных колебаний $q_0(t)=\mathcal{G}^{(1)}(t)$ и вынужденных $q(j;t)$. При этом нужно иметь ввиду, конечно, что движение не должно зависеть от источника в ненаступившем будущем, т. е. при $t>t''$, а также от того, что было до того, когда было задано исходное положение частицы, т. е. при $t<t'$, а значит, интеграл для вынужденных колебаний берется как определенный, т. е. в интервале $t'\leqslant t\leqslant t''$. Поскольку исходное уравнение для двухточечной функции 14.14 содержит оператор, симметричный по аргументам t_1 и t_2, и зависит от источника с аргументом t_1-t_2, его общее решение можно представить в виде частного решения неоднородного уравнения, зависящего, как и источник, от разности времени t_1-t_2, и общего решения однородного, которое симметрично относительно перестановки $t_1\leftrightarrow t_2$,

$$\mathcal{G}_{(12)}\left(t_1,t_2\right)=\tilde{\mathcal{G}}_{(12)}\left(t_1-t_2\right)+C\cdot\mathcal{G}_{(1)}\left(t_1\right)\mathcal{G}_{(1)}\left(t_2\right)$$

т. е. с точностью до вклада свободной волны с некоторой нормировкой C. Определить постоянную C можно, исходя из граничных условий: для свободных колебаний уже фиксированы условия $q_0\left(t'\right)=q'$ и $q_0\left(t''\right)=q''$, так что добавка к свободным вынужденных колебаний $q(j;t)$ должна подчиняться условиям

$$q\left(j;t'\right)=q\left(j;t''\right)\equiv 0$$

и следовательно, из явного вида вынужденных колебаний через двухточечную функцию 14.15 при произволъном источнике заключаем, что

$$\mathcal{G}_{(12)}\left(t',t\right)=\mathcal{G}_{(12)}\left(t'',t\right)=0,\quad t'\leqslant t\leqslant t'',$$

где мы учли, что $\mathcal{G}_{(12)}\left(t_1,t_2\right)$, как мы уже отмечали, должна быть симметрична по перестановке своих аргументов.

Задача 7.2.

Рассматривая решение уравнения 14.14 для двухточечной функции $\mathcal{G}_{(12)}\left(t_1,t_2\right)$ с заданными граничными условиями, докажите, что

$$\begin{aligned}\mathcal{G}_{(12)}\left(t_1,t_2\right)=\frac{1}{2m\omega_0\sin\omega_0\left(t''-t'\right)}\{&\sin\omega_0\left(t''-t'\right)\sin\omega_0\left|t_1-t_2\right|-\\&-\sin\omega_0\left(t_1-t'\right)\sin\omega_0\left(t''-t_2\right)-\\&-\sin\omega_0\left(t_2-t'\right)\sin\omega_0\left(t''-t_1\right)\},\end{aligned}$$

с учетом допустимого интервала значений $t'\leqslant t_{1,2}\leqslant t''$.

Точно так же при $n\geqslant 3$ уравнение Швингера-Дайсона означает, что

$$m\frac{\mathrm{d}^2}{\mathrm{d}t_1^2}\mathcal{G}_{(1\ldots n)}\left(t_1,\ldots,t_n\right)+m\omega_0^2\mathcal{G}_{(1\ldots n)}\left(t_1,\ldots,t_n\right)=0$$

и, следовательно, многоточечные функции Грина для осциллятора удовлетворяют свободному уравнению и могут быть построены в виде композиций $\mathcal{G}^{(1)}\left(t_k\right)$, что с учетом граничных условий (свободное движение уже включено в линейный вклад $\mathcal{G}_{(1)}\big)$ в виде

$\mathcal{G}_{(1...n)}(t_1,...,t_n)\big|_{t_k=t'} = \mathcal{G}_{(1...n)}(t_1,...,t_n)\big|_{t_k=t''} = 0, \quad t' \leqslant t_k \leqslant t'', \quad k = \{\overline{1,n}\}$,
приводит к результату

$$\mathcal{G}_{(1...n)}(t_1,...,t_n) = 0, \quad n \geqslant 3$$

Для осциллятора

$$G[j] = \mathcal{G}_0 + \int \mathcal{G}^{(1)}(t) j(t) \mathrm{d}t + \frac{1}{2!}\int \mathcal{G}_{(12)}(t_1,t_2)\, j(t_1)\, j(t_2)\, \mathrm{d}t_1\ \mathrm{d}t_2$$

Это есть исключительное свойство гармонического осциллятора - системы, гамильтониан которой квадратичен как по импульсу, так и по координате. Исключительное внимание к осциллятору обусловлено не столько тем, что задача решается точно, а в большей степени той ролью, которую осциллятор приобретает при рассмотрении полей: свободные поля представимы как сумма элементарных осцилляторов с волновым вектором $\boldsymbol{k}$ и частотой $\omega = \omega(\boldsymbol{k})$.

Амплитуду вероятности - матричный элемент оператора эволюции при наличии источников $-Z[j]$ также можно разложить в вариационный ряд Тейлора

$$Z[j] = 1 + \int \frac{\delta Z}{\delta j(t)}\bigg|_{j=0} j(t)\mathrm{d}t + \frac{1}{2!}\int \frac{\delta^2 Z}{\delta j(t_1)\,\delta j(t_2)}\bigg|_{j=0} j(t_1)\, j(t_2)\, \mathrm{d}t_1\ \mathrm{d}t_2 + \\ + \frac{1}{3!}\frac{\delta^3 Z}{\delta j_{(1)}\delta j_{(2)}\delta j_{(3)}}\bigg|_{j=0} j_{(1)} j_{(2)} j_{(3)} + ...$$

где мы отнормировали амплитуду на единицу, как это уже было описано выше. Это разложение записывают через кореляторы. Так,

$$-\,\mathrm{i}\hbar\frac{\delta Z}{\delta j(t)}\bigg|_{j=0} = \langle \hat{q}(t)\rangle = \mathcal{G}^{(1)}(t)$$

где усреднение берется то начальному и конечному состоянию, заданным в задаче, так что одноточечный коррелятор - это матричный элемент координаты, а в случае переходов «вакуум-вакуум» - это среднее значение координаты по вакууму. Далее, во втором порядке по внешним источникам возникает величина

$$(-\mathrm{i}\hbar)^2\frac{\delta^2 Z}{\delta j(t_1)\,\delta j(t_2)}\bigg|_{j=0} = \left\langle \hat{T}\left\{\hat{q}(t_1)\,\hat{q}(t_2)\right\}\right\rangle$$

которая есть двухточечный коррелятор, который еще называют пропагатором, а в высших порядках вводят

$$\mathcal{D}_{(1...n)} = (-\mathrm{i}\hbar)^n\frac{\delta^n Z}{\delta j_{(1)}...\delta j_{(n)}}\bigg|_{j=0} = \left\langle \hat{\mathrm{T}}\left\{\hat{q}(t_1)...\hat{q}(t_n)\right\}\right\rangle$$

который называют n-точечным коррелятором (на жаргоне «n-точка»). Значит,

$$Z[j] = \sum_{n=1}^{\infty}\left(\frac{\mathrm{i}}{\hbar}\right)^n \frac{1}{n!}\mathcal{D}_{(1...n)} j_{(1)}...j_{(n)}.$$

Для двухточечной функции $\mathcal{D}_{(12)}$ в самом общем случае имеем

$$\mathcal{D}_{(12)}(t_1,t_2) = -\mathrm{i}\hbar\mathcal{G}_{(12)}(t_1,t_2) + \mathcal{G}^{(1)}(t_1)\,\mathcal{G}^{(1)}(t_2)$$

В случае переходов «вакуум-вакуум» для осциллятора $\mathcal{G}^{(1)}(t) \equiv 0$, так что можно однозначно вычислить двухточечные функции $\mathcal{D}_{(12)}$ и $\mathcal{G}_{(12)}$. В самом деле, уравнение Швингера-Дайсона 14.9 в случае осциллятора имеет вид

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\left\{-\mathrm{i}\hbar\frac{\delta Z[j]}{\delta j(t)}\right\} = -m\omega_0^2(-\mathrm{i}\hbar)\frac{\delta}{\delta j(t)}Z[j] + j(t)Z[j]$$

так что, если взять вариационную производную по источникам $j\,(t_2)$ и положить $j = 0$, то получится

$$m\left\{\frac{\mathrm{d}^2}{\mathrm{d}t_1^2} + \omega_0^2\right\}(-\mathrm{i}\hbar)^2\frac{\delta^2 Z}{\delta j_{(1)}\delta j_{(2)}}\bigg|_{j=0} = -\mathrm{i}\hbar\delta\,(t_1 - t_2)\,.$$

Поскольку

$$(-\mathrm{i}\hbar)^2\frac{\delta^2 Z}{\delta j_{(1)}\delta j_{(2)}}\bigg|_{j=0} = \mathcal{D}_{(12)} = \left\langle 0\,\middle|\hat{\mathrm{T}}\left\{\hat{q}\,(t_1)\,\hat{q}\,(t_2)\right\}\middle|\,0\right\rangle$$

находим уравнение на функцию Грина $\mathcal{D}_{(12)}$

$$m\left\{\frac{\mathrm{d}^2}{\mathrm{d}t_1^2} + \omega_0^2\right\}\mathcal{D}_{(12)} = -\mathrm{i}\hbar\delta\,(t_1 - t_2)\,.$$

Записывая преобразование Фурье

$$\mathcal{D}_{(12)}(t) = \int\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-\mathrm{i}\omega t}\mathcal{D}^{(2)}(\omega)$$

найдем, что

$$\mathcal{D}^{(2)}(\omega) = \frac{\mathrm{i}\hbar}{m\,(\omega^2 - \omega_0^2)}$$

имеет полюса при $\omega = \pm\omega_0$, обход которых должен быть согласован с граничными условиями в асимптотическом прошлом и будущем. Решение в виде контура интегрирования в плоскости комплексной ω показано на рис. 21.

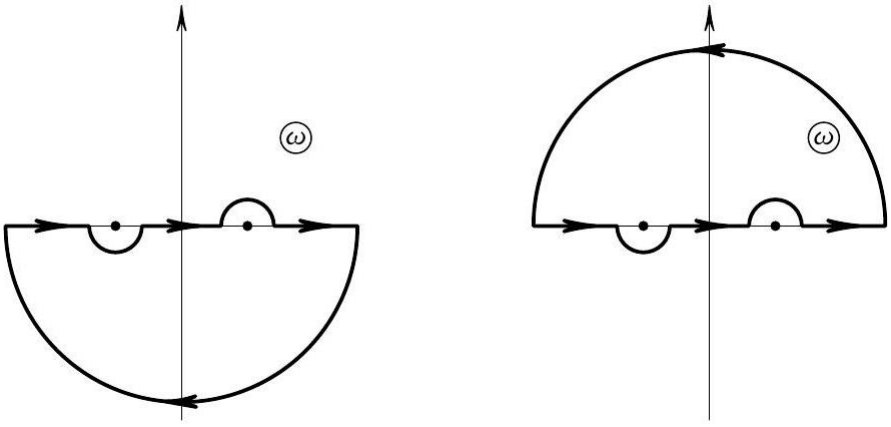


Рис. 21. Контуры интегрирования в плоскости комплексной переменной ω при $t \to +\infty$ (слева) и $t \to -\infty$ (справа)

В самом деле, при $t \to +\infty$ контур можно замкнуть в нижней полуплоскости, так как отрицательная мнимая добавка к частоте в экспоненте приводит к нулевому вкладу по полуокружности, и полюс при $\omega = \omega_0 - \mathrm{i}0$ в экспоненте дает положительно частотную моду. Аналогично, при $t \to -\infty$ вклад по полуокружности в верхней полуплоскости обращается в нуль, и полюс при $\omega = -\omega_0 + \mathrm{i}0$ дает отрицательно частотную моду.

В итоге получаем так называемую причинную двухточечную фейнмановскую функиию Грина, которую такюе называют пропагатором:

$$\mathcal{D}^{(2)}(\omega) = \frac{\mathrm{i}\hbar}{m}\frac{1}{\omega^2 - \omega_0^2 + \mathrm{i}0}.$$

Описанные граничные условия, очевидно, можно получить, заметив, что они выводятся посредством замены $\omega_0 \to \omega_0(1 - \mathrm{i}\varepsilon)$, где $\varepsilon \to +0$, т. е. добавкой бесконечно малого затухания. Мы видели, что это затухание связано с шириной резонанса. Поэтому ясно, что физически малое значение ε приводит к вымиранию возбуждений вакуума, т. е. следует из условия стабильности вакуума. Этот же аргумент приводит к математическому обоснованию поворота Вика в плоскости частот (соответствующие интегралы по контуру при вращении от вещественной оси к мнимой на угол $\pi/2$ не встречают полюсов).

После преобразования Фурье

$$\mathcal{D}_{(12)}(t) = \int\limits_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{2\pi} \cdot \mathrm{e}^{-\mathrm{i}\omega t} \mathcal{D}^{(2)}(\omega)$$

которое можно найти, взяв при $t > 0$ интеграл Коши по контуру, изображенному слева на рис. 21.

$$\mathcal{D}_{(12)}(t) = \frac{\hbar}{2\omega_0 m} \mathrm{e}^{-\mathrm{i}\omega_0 t}, \quad t > 0$$

и при $t < 0$ по контуру справа на рис. 21

$$\mathcal{D}_{(12)}(t) = \frac{\hbar}{2\omega_0 m} \mathrm{e}^{\mathrm{i}\omega_0 t}, \quad t < 0$$

получаем

$$\mathcal{D}_{(12)}(t) = \frac{\hbar}{2\omega_0 m} \mathrm{e}^{-i\omega_0 |t|}$$

Этот же результат был получен нами операторным методом (см. стр. 257 раздел 13.2.

Задача 7.3. Методом выделения гауссовых вкладов и замены переменной интегрирования в фейнмановском интеграле по траекториям показать, что квадратичное по траектории действие вида

$$S\left(t', q', t'', q''\right) = \frac{1}{2} \int\limits_{t', q'}^{t'', q''} \mathrm{d}t q(t) \hat{\Gamma} q(t) + \int\limits_{t', q'}^{t'', q''} \mathrm{d}t j(t) q(t),$$

где оператор эволюции является эрмитово самосопряженным, $\hat{\Gamma} = \hat{\Gamma}^{\dagger}$, например, для осциллятора $\hat{\Gamma} q(t) = -m \left\{ \mathrm{d}^2 q(t)/\mathrm{d}t^2 + \omega_0^2 q(t) \right\}$, приводит к производящему функционалу связных функций Грина

$$G[j] = \mathcal{G}_0 + \int \mathcal{G}^{(1)}(t) j(t) \mathrm{d}t + \frac{1}{2!} \int \mathcal{G}^{(2)}\left(t_1, t_2\right) j\left(t_1\right) j\left(t_2\right) \mathrm{d}t_1 \, \mathrm{d}t_2$$

в котором $\mathcal{G}^{(1)}(t)$ - решение однородного уравнения

$$\hat{\Gamma} \mathcal{G}^{(1)}(t) = 0$$

с граничными условиями $\mathcal{G}^{(1)}\left(t'\right) = q', \mathcal{G}^{(1)}\left(t''\right) = q''$, а

$$\hat{\Gamma}^{-1} j\left(t_1\right) = -\int \mathcal{G}^{(2)}\left(t_1, t_2\right) j\left(t_2\right) \mathrm{d}t_2.$$

Задача 7.4. Докажите, что для симметричной вещественной матрицы M с положительными собственными значениями кратный гауссов интеграл

$$\int \exp\left\{-q_\alpha M^\alpha_\beta q^\beta\right\} \prod_{\alpha=1}^{n} \mathrm{d}q^\alpha = \frac{\pi^{n/2}}{\sqrt{\det M}}$$

Решение. У равнение на собственные значения матрицы

$$M \cdot e_k = \lambda_k e_k$$

задает базис собственных векторов матрицы, так что обратимое преобразование от координат q координатам $\tilde{q}$ в базисе e_k

$$q^\alpha = \mathcal{R}^\alpha_\beta \tilde{q}^\beta$$

приводит матрицу M к диагональному виду

$$\mathcal{R}^{\mathrm{T}} \cdot M \cdot \mathcal{R} = \mathrm{diag}\,(\lambda_1, ..., \lambda_n)$$

причем

$$\det M = \frac{1}{(\det \mathcal{R})^2} \prod_{k=1}^{n} \lambda_k$$

Тогда замена переменных интегрирования дает

$$\int \det \mathcal{R} \prod_{k=1}^{n} \mathrm{d}\tilde{q}_k \exp\left\{-\tilde{q}_k^2 \lambda_k\right\} = \det \mathcal{R} \prod_{k=1}^{n} \sqrt{\frac{\pi}{\lambda_k}} = \frac{\pi^{n/2}}{\sqrt{\det M}}$$

Заметим, что для вещественной симметричной матрицы M приведение к базису собственных векторов производится ортогональной матрицей, так что $\det \mathcal{R} = 1$, и детерминант сводится к произведению собственных значений матрицы M.

Задача 7.5. Для гармонического осциллятора вычислить интеграл по траекториям с граничными условиями $q\,(t') = q\,(t'') = 0$. Использовать известное выражение для интеграла по траекториям для свободной частицы и представление детерминанта в виде произведения собственных значений.

Решение. Интеграл

$$Z = \mathcal{N} \int \mathcal{D}q \exp\left\{-\frac{\mathrm{i}}{\hbar}\frac{m}{2}\int_{t'}^{t''} \mathrm{d}t q(t) \left(\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \omega_0^2\right) q(t)\right\}\Bigg|_{q'=q''=0}$$

относится к гауссову типу с операторной матрицей

$$\hat{M} = \frac{m}{2}\left(\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \omega_0^2\right)$$

которая при решении уравнения на собственные значения

$$\hat{M} q(t) = \lambda q(t), \qquad \text{при } q\,(t') = q\,(t'') = 0$$

имеет собственные функции

$$q(t) = \tilde{q} \sin \frac{\pi n\,(t - t')}{t'' - t'}, \quad n \geqslant 1$$

Так чТО

$$\lambda_n = -\frac{m}{2}\left\{\left(\frac{\pi n}{t''-t'}\right)^2 - \omega_0^2\right\}$$

После поворота Вика $t''-t' = -\mathrm{i}\Delta t_E$ собственные значения становятся положительНЫМи

$$\lambda_{E,n} = \frac{m}{2}\left(\frac{\pi n}{\Delta t_E}\right)^2\left\{1+\left(\frac{\omega_0\Delta t_E}{\pi n}\right)^2\right\}$$

а значит, функциональный детерминант операторной матрицы

$$\mathrm{Det}\,\hat{M} = \prod_{n=1}^{\infty}\lambda_{E.n} = \mathrm{Det}\,\hat{M}_0\prod_{n=1}^{\infty}\left\{1+\left(\frac{\omega_0\Delta t_E}{\pi n}\right)^2\right\}$$

где $\hat{M}_0 = \lim_{\omega_0\to 0}\hat{M}$ - это операторная матрица свободной частицы. Тогда, используя связь гауссова интеграла с детерминантом матрицы, в случае с интегралом по траекториям находим, что искомый интеграл

$$Z = \mathcal{N}\int \mathcal{D}q\exp\left\{-\frac{\mathrm{i}}{\hbar}\frac{m}{2}\int_{t'}^{t''}\mathrm{d}t q(t)\frac{\mathrm{d}^2}{\mathrm{d}t^2}q(t)\right\}\Bigg|_{q'=q''=0}\cdot\frac{1}{\sqrt{\prod_{n=1}^{\infty}\left\{1+\left(\frac{\omega_0\Delta t_E}{\pi n}\right)^2\right\}}}.$$

Мы уже вычислили интеграл по траекториям для свободной частицы, который в случае нулевых значений $q'=q''=0$ равен

$$Z_0 = \mathcal{N}\int \mathcal{D}q\exp\left\{-\frac{\mathrm{i}}{\hbar}\frac{m}{2}\int_{t'}^{t''}\mathrm{d}t q(t)\frac{\mathrm{d}^2}{\mathrm{d}t^2}q(t)\right\}\Bigg|_{q'=q''=0} = \sqrt{\frac{m}{2\pi\hbar\Delta t_E}}.$$

С учетом формуль [1]

$$\prod_{n=1}^{\infty}\left\{1+\left(\frac{z}{\pi n}\right)^2\right\} = \frac{\mathrm{sh}\,z}{z}$$

находим

$$Z = \sqrt{\frac{m}{2\pi\hbar\Delta t_E}}\sqrt{\frac{\omega_0\Delta t_E}{\mathrm{sh}\,\omega_0\Delta t_E}} = \sqrt{\frac{-\mathrm{i}m\omega_0}{2\pi\hbar\sin\omega_0\left(t''-t'\right)}}$$

Задача 7.6. Для осциллятора с источником покажите, что интеграл по траекториям имеет вид

$$Z = \sqrt{\frac{-\mathrm{i}m\omega_0}{2\pi\hbar\sin\omega_0\left(t''-t'\right)}}\exp\left\{\frac{\mathrm{i}}{\hbar}S_{\mathrm{cl}}\left(t'',t',j\right)\right\}$$

где S_{cl} - действие на траектории $q_{\mathrm{cl}}(t)$ с источником,

$$m\left\{\ddot{q}_{\mathrm{cl}}(t)+\omega_0^2 q_{\mathrm{cl}}(t)\right\} = j(t),\quad q_{\mathrm{cl}}\left(t'\right)=q',\quad q_{\mathrm{cl}}\left(t''\right)=q''.$$

Используйте замену переменной интегрирования $q(t)\mapsto y(t)$,

$$q(t) = q_{\mathrm{cl}}(t)+y(t),\quad y\left(t'\right)=y\left(t''\right)=0.$$

Теорема Вика. В случае рассмотрения вакуум-вакуумных переходов для затравочного действия (bare action), квадратичного по координатам, в формализме интеграла по траекториям легко получить выражение для функции Грина функционала $Z[j]$

$$\mathcal{D}^{(n)}\left(t_1,...,t_n\right)=\left\langle \mathrm{in}\left|\hat{\mathrm{T}}\left\{\hat{q}\left(t_1\right)...\hat{q}\left(t_n\right)\right\}\right|\mathrm{in}\right\rangle$$

[1] В теории функций комплексной переменной доказывается, что целая функция $f(z)$ может быть построена как произведение полиномов первого порядка с узлами, которые расположены точно в узлах $z_n\neq 0$ функции $f(z)$:

$$f(z)=f(0)\prod_{n=-\infty}^{\infty}\left\{1-\frac{z}{z_n}\right\}$$

В случае $f(z)=\mathrm{sh}\,z/z$ разложение в ряд Тейлора гиперсинуса по нечетным степеням z показывает, что мы имеем дело с целой функцией, узлы которой $z_n=\mathrm{i}\pi n$. Тогда умножение сомножителей с противоположными значениями n

$$\left\{1-\frac{z}{\mathrm{i}\pi n}\right\}\left\{1+\frac{z}{\mathrm{i}\pi n}\right\}=\left\{1+\left(\frac{z}{\pi n}\right)^2\right\}$$

дает суммирование по $n\geqslant 1$, а $f(0)=1$ сразу воспроизводит формулу 14.23. где мы опустили индекс, обозначающий представление Гейзенберга для операторов, зависящих от времени. Напомним краткие обозначения «интегрирования по паре немых индексов», так что, например,

$$j_{(1)}q_{(1)}\cong\int \mathrm{d}t_1 j\left(t_1\right)q\left(t_1\right),\quad j_{(1)}\mathcal{G}_{(12)}j_{(2)}\cong\int \mathrm{d}t_1\ \mathrm{d}t_2 j\left(t_1\right)\mathcal{G}_{(12)}\left(t_1,t_2\right)j\left(t_2\right).$$

Тогда для квадратичного действия, как мы видели,

$$Z[j]=\exp\left\{\frac{\mathrm{i}}{\hbar}\frac{1}{2}j_{(t)}\mathcal{G}_{(tt')}j_{(t')}\right\}=\exp\left\{-\frac{1}{\hbar^2}\frac{1}{2}j_{(t)}\mathcal{D}_{(tt')}j_{(t')}\right\}$$

Заметим, что для функционала $F[j]$, который разлагается в сходящийся вариационный ряд Тейлора, имеет место соотношение,

$$j(t)=-\mathrm{i}\hbar\frac{\delta}{\delta\phi(t)}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}j_{(\tilde{t})}\tilde{\phi}_{(\tilde{t})}}\Big|_{\tilde{\phi}=0}\quad\Rightarrow\quad F[j]=F\left[-\mathrm{i}\hbar\frac{\delta}{\delta\phi}\right]\mathrm{e}^{\frac{\mathrm{i}}{\hbar}j_{(\tilde{t})}\tilde{\phi}_{(\tilde{t})}}\Big|_{\phi=0}.$$

Используя этот трюк, сразу найдем

$$Z[j]=\exp\left\{\frac{1}{2}\mathcal{D}_{(tt')}\frac{\delta^2}{\delta\phi_{(t)}\delta\phi_{(t')}}\right\}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}j_{(\tilde{t})}\phi_{(\tilde{t})}}\Big|_{\phi=0}$$

Для n-точечного коррелятора находим

$$\mathcal{D}_{(1...n)}=(-\mathrm{i}\hbar)^n\frac{\delta^n Z[j]}{\delta j_{(1)}...\delta j_{(n)}}\Big|_{j=0}=\exp\left\{\frac{1}{2}\mathcal{D}_{(tt')}\frac{\delta^2}{\delta\phi_{(t)}\delta\phi_{(t')}}\right\}\phi_{(1)}...\phi_{(n)}\Big|_{\phi=0},$$

и при нечетном $n=2p+1$, очевидно, $\mathcal{D}_{(1...n)}=0$. Введем понятие «спаривания полей»

$$\underbrace{\phi_{(k)}\phi_{(k')}}\cong\mathcal{D}_{(kk')}=-\mathrm{i}\hbar\mathcal{G}_{(kk')}.$$

Тогда при четном $n=2p$ функция Грина $\mathcal{D}_{(1...n)}$ сводится к сумме всевозможных спариваний полей [1]

$$\mathcal{D}_{(1\ldots n)} = \sum_{\substack{\text{все варианты}\\ \text{спаривания}}} \underbrace{\phi_{(k)}\phi_{(k')}} \cdots \underbrace{\phi_{(l)}\phi_{(l')}}, \quad k \neq k', l \neq l' \in \overline{\{1,n\}},$$

что и составляет суть теоремы Вика.

Пример двухточечного корреляторы мы уже рассмотрели. А для четырехточечного коррелятора мы получим 3 варианта спаривания, каждое из которых отвечает распространению кванта между точками в аргументе коррелятора,

$$\mathcal{D}_{(1234)} = \underbrace{\phi_{(1)}\phi_{(2)}}\underbrace{\phi_{(3)}\phi_{(4)}} + \underbrace{\phi_{(1)}\phi_{(3)}}\underbrace{\phi_{(2)}\phi_{(4)}} + \underbrace{\phi_{(1)}\phi_{(4)}}\underbrace{\phi_{(2)}\phi_{(3)}},$$

[1] Множитель $1/2$ в аргументе экспоненты с вариационными производными второго порядка всегда компенсируется двумя способами выбора первого и второго поля в спаривании. так что графически

В этом случае диаграммы не являются связными.

2. Теория возмущений. При введении в действие полиномиального взаимодействия по полям степени выше 2

$$S_{\text{int}}\left[q\right] = -\int \mathrm{d}t V_{\text{int}}\left(q(t)\right)$$

можно использовать ту же методику спаривания полей. Для этого сначала заметим, что экспоненту с $S_{\text{int}}\left[q\right]$ можно вынести из-под интеграла по траекториям, сделав подстановку

$$q \mapsto -\mathrm{i}\hbar\frac{\delta}{\delta j}, \quad \Rightarrow \quad S_{\text{int}}[q] \mapsto S_{\text{int}}\left[-\mathrm{i}\hbar\frac{\delta}{\delta j}\right]$$

так что действие под интегралом S включает в себя только действие для свободного осциллятора

$$S_0[q] = -\int \mathrm{d}t q(t)\left\{m\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \omega_0^2\right\}q(t)$$

и вклад от внешнего источника

$$S_{\text{ext}}[j] = \int \mathrm{d}t j(t)q(t)$$

$S = S_0 + S_{\text{ext}}$, а значит, можно провести интегрирование и получить амплитуду вероятности квантовых переходов при наличии источников

$$Z[j] = \exp\left\{\frac{\mathrm{i}}{\hbar}S_{\text{int}}\left[-\mathrm{i}\hbar\frac{\delta}{\delta j}\right]\right\}\exp\left\{-\frac{1}{\hbar^2}\frac{1}{2}j_{(t)}\mathcal{D}_{(tt')}j_{(t')}\right\}.$$

Тогда трюк с ведением вариационных производных экспоненты

$$\mathrm{e}^{\frac{\mathrm{i}}{\hbar}j_{(\tilde{t})}\phi_{(\tilde{t})}}$$

по вспомогательному полю ϕ позволяет провести дальнейшие преобразования с помощью подстановок

$$-\mathrm{i}\hbar\frac{\delta}{\delta j}\mapsto\phi,\quad j\mapsto-\mathrm{i}\hbar\frac{\delta}{\delta\phi}$$

и получить

$$Z[j]=\exp\left\{\frac{1}{2}\mathcal{D}_{(tt')}\frac{\delta^2}{\delta\phi_{(t)}\delta\phi_{(t')}}\right\}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left\{S_{\mathrm{int}}[\phi]+j_{(\tilde{t})}\phi_{(\tilde{t})}\right\}}\Bigg|_{\phi=0}.$$

Значит, для многоточечной амплитуды находим

$$\mathcal{D}_{(1\ldots n)}=\exp\left\{\frac{1}{2}\mathcal{D}_{(tt')}\frac{\delta^2}{\delta\phi_{(t)}\delta\phi_{(t')}}\right\}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S_{\mathrm{int}}[\phi]}\phi_{(1)}\ldots\phi_{(n)}\Bigg|_{\phi=0}.$$

В этом выражении нужно учитывать все спаривания полей, включая поля в S_{int} . Формула 14.29 представляет собой основу для построения теории возмущений, поскольку все многоточечные функции выражаются через спаривания «свободных» полей, часть из которых возникает при разложении экспоненты с действием взаимодействия. В свою очередь, действие взаимодействия обычно включает в себя полиномы по полям с коэффициентами - константами взаимодействия.

Пример взаимодействия - потенциал

$$V_{\mathrm{int}}\ =\frac{1}{3!}\Lambda q^3$$

где Λ постоянная, которая имеет размерность массы, деленной на длину и квадрат времени. Тогда в первом порядке по Λ трехточечный коррелятор

$$\mathcal{D}_{(123)}=\exp\left\{\frac{1}{2}\mathcal{D}_{(tt')}\frac{\delta^2}{\delta\phi_{(t)}\delta\phi_{(t')}}\right\}\left\{-\frac{\mathrm{i}}{\hbar}\frac{1}{3!}\Lambda\int\mathrm{d}\tilde{t}\phi^3(\tilde{t})\right\}\phi_{(1)}\phi_{(2)}\phi_{(3)}\Bigg|_{\phi=0}.$$

В этой формуле есть вклад, когда спаривание происходит между «полями» с внешними временами $\phi_{(1)},\phi_{(2)},\phi_{(3)}$ и «полем» $\phi(\tilde{t})$, и такое спаривание имеет 3 ! вариантов. Есть вклад, когда два поля с внешними временами спариваются между собой, а третье - с одним из трех полей $\phi(\tilde{t})$(3 варианта). В итоге,

$$\begin{aligned}\mathcal{D}_{(123)}=&-\frac{\mathrm{i}}{\hbar}\Lambda\mathcal{D}_{(1\tilde{t})}\mathcal{D}_{(2\tilde{t})}\mathcal{D}_{(3\tilde{t})}-\\&-\frac{\mathrm{i}}{\hbar}\frac{\Lambda}{2}\left\{\mathcal{D}_{(12)}\mathcal{D}_{(3\tilde{t})}\mathcal{D}_{(\tilde{t}\tilde{t})}+\mathcal{D}_{(13)}\mathcal{D}_{(3\tilde{t})}\mathcal{D}_{(\tilde{t}\tilde{t})}+\mathcal{D}_{(23)}\mathcal{D}_{(1\tilde{t})}\mathcal{D}_{(\tilde{t}\tilde{t})}\right\}\end{aligned}$$

В этой формуле по повторяющемуся немому индексу $\tilde{t}$ в скобках согласно введенному нами правилу ведется интегрирование. Следуя теперь уже обоснованному и введенному выше правилу изображения двухточечного коррелятора в виде прямой, соединяющей 2 точки в аргументе коррелятора, получим диаграмму Фейнмана, которая изображена на рис. 22 и отвечает выражению 14.31. Подчеркнем, что взаимодействие, которое записывается

Рис. 22. Диаграммы для трехточечной функции Грина в модели с потенциалом 14.30, которую называют «лямбда-фи-в-кубе». (Для краткости записи множителей на рисунке мы положили $\hbar=1$.

как интеграл, приводит к тому, что в теории возмущений пропагаторы квантов сходятся в одной точке, указанной в аргументе интеграла в действии взаимодействия. Говорят, что взаимодействие соответствует вершинам взаимодействия квантов, поскольку без него пропагаторы соединяли бы только внешние точки в аргументе корреляторов (функций Грина). Ясно, что это позволяет ввести понятие внешних и внутренних линий: у внешних есть точка из аргумента коррелятора, а у внутренних нет таких точек. Кроме того, естественно ввести и понятие числа компонент связности диаграммы Фейнмана как число непрерывных цепочек из внутренних и внешних линий на диаграмме. На рис. 22 все диаграммы содержат по одной вершине, в первой одна компонента свзности, во второй -2 компоненты.

Подчеркнем, что в рассмотренном нами простом случае, когда нет вакуумных полей, т. е. $\mathcal{G}^{(1)} \equiv 0$, вклад вакуумных амплитуд

$$\mathcal{D}_0 = \exp\left\{\frac{1}{2}\mathcal{D}_{(tt')}\frac{\delta^2}{\delta\phi_{(t)}\delta\phi_{(t')}}\right\} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S_{\mathrm{int}}\,[\phi]}\Big|_{\phi=0},$$

очевидно, факторизуется для всех многоточечных функций в виде суммы всех диаграмм без внешних концов.

8.2.3 Diagrams in the Kiselev Formalism

(это не такой распространенный формализм, следует относиться к нему как просто к иллюстрации, что так можно делать. и этот раздел нужно переписать, у Киселева очень непонятно все написано!!!)

Теория

После рассмотрения примеров в теории возмущений, когда диаграммы имеют вполне определенный смысл в виде формул имеет смысл ввести графические обозначения и для вкладов в вариационный ряд Тейлора. Например, подынтегральные выражения в разложении функционала $G[j]$

$$\begin{aligned} G[j] =& \mathcal{G}_0 + \int \mathcal{G}^{(1)}(t) j(t) \mathrm{d}t + \\ &+ \frac{1}{2!}\int \mathcal{G}^{(2)}\left(t_1, t_2\right) j\left(t_1\right) j\left(t_2\right) \mathrm{d}t_1\ \mathrm{d}t_2 + \ldots = \sum_{n=0}^{\infty} \mathcal{G}_{(1\ldots n)} \frac{1}{n!} j_{(1)} \cdots j_{(n)}. \end{aligned}$$

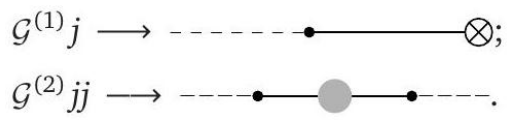
принято изображать в виде рисунков, строго соответствующих определенным выражениям, или, как говорят, в виде диаграмм Фейнмана согласно правилам:

1. источнику $j\left(t_k\right)$ сопоставляется луч, показанный штриховой линией с началом в точке t_k;

2. одноточечной функции Грина $\mathcal{G}^{(1)}\left(t_k\right)$ сопоставляется знак окружности вокруг креста в центре, т. е. $\otimes$, из которого исходит отрезок, показанный сплошной линией, с концом в точке t_k, причем метка крестом символизирует зависимость от граничных условий;

3. многоточечная функция Грина $\mathcal{G}_{(1\ldots n)}\left(t_1, \ldots, t_n\right)$ изображается окружностью с исходящими из нее n отрезками, показанными сплошной линией, причем каждому отрезку соответствует конец в одной из точек $t_1, \ldots, t_n$.

Например, в разложении функционала $G[j]$ для свободного осциллятора есть только два вклада 1



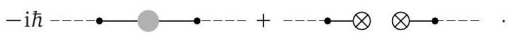
[1] Для краткости на диаграмме мы используем символ $\mathcal{G}^{2)} \equiv \mathcal{G}_{(12)}$ для двухточечной функции. В общем случае $G[j]$ называют прочзводящим функиионалом для связных функций Грина $\mathcal{G}_{(1\ldots n)}$, так как по построению в нем не содержатся вклады, которые можно представить в виде произведения интегральных множителей, которым соответствуют диаграммы Фейнмана, не соединенные никакими линиями 1. Если же рассмотреть разложение функционала $Z[j]$

$$Z[j] = \mathcal{D}_0 + \mathrm{i}/\hbar \int \mathcal{D}^{(1)}(t) j(t) \mathrm{d}t + \frac{(\mathrm{i}/\hbar)^2}{2!} \int \mathcal{D}^{(2)}\left(t_1, t_2\right) j\left(t_1\right) j\left(t_2\right) \mathrm{d}t_1 \, \mathrm{d}t_2 + \ldots$$

то в нем, несомненно, есть факторизуемые вклады, так как $Z[j] = \exp\left[\frac{\mathrm{i}G[j]}{\hbar}\right]$. Действительно, для двухточечной функции $\mathcal{D}$ имеем

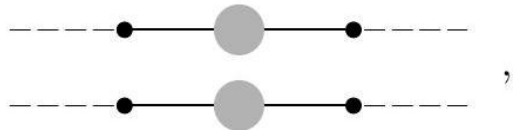
$$\mathcal{D}_{(12)}\left(t_1, t_2\right) = -\mathrm{i}\hbar \mathcal{G}^{(2)}\left(t_1, t_2\right) + \mathcal{G}^{(1)}\left(t_1\right) \mathcal{G}^{(1)}\left(t_2\right)$$

чему соответствует диаграмма



Очевидно, что вторая диаграмма не является связной (у нее есть разрыв).

Точно так же четырехточечная функция $\mathcal{D}$ может быть представлена, в частности, вкладами произведений $\mathcal{G}^{(2)}\mathcal{G}^{(2)}$ с различными комбинациями аргументов, что дает члены типа



т. е. опять же несвязные диаграммы.

Более подробно вопрос о связных вкладах в производящем функционале функций Грина можно сформулировать следующим образом:

прежде всего для того, чтобы факторизовать величину $Z[j]$ при нулевых источниках, а заодно и нормировочный множитель $\mathcal{N}$, который не зависит от источников, вводят $\tilde{Z}[j] = Z[j]/Z[0]$. Тогда разложение в ряд по источникам начинается с единицы:

$$\tilde{Z}[j] = 1 + \sum_{k=1}^{\infty} \left(\frac{\mathrm{i}}{\hbar}\right)^k \int \mathcal{D}_{(1\ldots k)}\left(t_1, \ldots, t_k\right) \frac{1}{k!} \prod_{k'=1}^{k} j\left(t_{k'}\right) \mathrm{d}t_{k'}.$$

В функциях Грина $\mathcal{D}$, как мы видели, есть несвязные вклады, что соответствует произведениям связных функций $\mathcal{D}^c[c = \text{connected}]$, которые уже не распадаются на произведения других связных функций. Для краткости обозначений запишем k-точечные связные вклады в виде

$$a_k = \left(\frac{\mathrm{i}}{\hbar}\right)^k \int \mathcal{D}^c_{(1\ldots k)}\left(t_1, \ldots, t_k\right) \frac{1}{k!} \prod_{k'=1}^{k} j\left(t_{k'}\right) \mathrm{d}t_{k'}.$$

Тогда связные компоненты в выражении для амплитуды $\tilde{Z}[j]$ можно сгруппировать не по числу внешних токов, а так, чтобы выразить через них

[1] Доказательство мы приведем ниже. все несвязные диаграммы следующим образом: каждый k-точечный связный вклад a_k может повториться в несвязной диаграмме n_k раз, но сумма n_k фиксирует число компонент связности в диаграмме, а значит, суммирование диаграмм по числу компонент связности N примет вид

$$\tilde{Z}[j] = 1 + \sum_{N=1}^{\infty} \sum_{n_k} \left(\prod_{k=1}^{\infty} \frac{1}{(n_k)!} a_k^{n_k} \right) \Bigg|_{\sum n_k = N},$$

где N - число произведений связных вкладов, т. е. число компонент связности в диаграмме, а n_k - количество вкладов с k-точечными связными функциями Грина, которые входят симметрично и, стало быть, допускают (n_k) ! перестановок, дающих одинаковые вклады, причем $\sum n_k = N$.

Заметим теперь, что разложение экспоненты в ряд

$$\exp a_1 = 1 + \sum_{N=1}^{\infty} \sum_{n_1} \left(\prod_{k=1}^{1} \frac{1}{(n_1)!} a_1^{n_1} \right) \Bigg|_{n_1 = N}$$

для двух слагаемых принимает вид

$$\exp\{a_1 + a_2\} = 1 + \sum_{N=1}^{\infty} \sum_{n_1, n_2} \left(\prod_{k=1}^{2} \frac{1}{(n_k)!} a_k^{n_k} \right) \Bigg|_{n_1 + n_2 = N}$$

и, как нетрудно сообразить,

$$\exp\left\{ \sum_{k=1}^{\infty} a_k \right\} = 1 + \sum_{N=1}^{\infty} \sum_{n_k} \left(\prod_{k=1}^{\infty} \frac{1}{(n_k)!} a_k^{n_k} \right) \Bigg|_{\sum n_k = N}$$

Таким образом, мы показали, что факторизация несвязных амплитуд в произведение связных действительно приводит к экспоненциированию связных амплитуд, и подстановка $Z[j] = \exp\{\mathrm{i}G[j]/\hbar\}$ - это переход к производящему функционалу связных функций Грина $G[j]$. Этот вывод справедлив и при наличии ненулевых вакуумных значений $\langle q \rangle$, поскольку вклад вакуума факторизован в $Z[0]$.

Ситуация с разложением производящего функционала и, следовательно, со множеством допустимых диаграмм существенно изменяется, если ввести ангармоничность осциллятора. Для определенности, пусть

$$V(q) = V_0(q) + V_{\text{int}}(q) = \frac{m\omega_0^2}{2} q^2 + \frac{\lambda}{4!} q^4$$

где λ - постоянная, задающая степень ангармоничности. Тогда в уравнении Швингера-Дайсона вклад потенциала задается величиной

$$
\begin{aligned}
&\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}G[j]}V'_{\mathrm{int}}\left(-\mathrm{i}\hbar\frac{\delta}{\delta j(t)}\right)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}G[j]} = \frac{\lambda}{3!}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}G[j]}(-\mathrm{i}\hbar)^3\frac{\delta^3}{\delta j(t)^3}\left\{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}G[j]}\right\} = \\
&= \mathrm{i}\hbar^3\frac{\lambda}{3!}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}G[j]}\frac{\delta^2}{\delta j(t)^2}\left\{\frac{\mathrm{i}}{\hbar}\frac{\delta G}{\delta j}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}G[j]}\right\} = \\
&= \mathrm{i}\hbar^3\frac{\lambda}{3!}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}G[j]}\frac{\delta}{\delta j(t)}\left\{\left[\frac{\mathrm{i}}{\hbar}\frac{\delta^2 G}{\delta j^2} - \frac{1}{\hbar^2}\left(\frac{\delta G}{\delta j}\right)^2\right]\mathrm{e}^{\frac{\mathrm{i}}{\hbar}G[j]}\right\} = \\
&= \mathrm{i}\hbar^3\frac{\lambda}{3!}\left\{\frac{\mathrm{i}}{\hbar}\frac{\delta^3 G}{\delta j^3} - \frac{3}{\hbar^2}\frac{\delta G}{\delta j}\frac{\delta^2 G}{\delta j^2} - \frac{\mathrm{i}}{\hbar^3}\left(\frac{\delta G}{\delta j}\right)^3\right\} = \\
&= \frac{\lambda}{6}\left(\frac{\delta G}{\delta j}\right)^3 - \frac{\lambda}{2}\mathrm{i}\hbar\frac{\delta G}{\delta j}\frac{\delta^2 G}{\delta j^2} - \frac{\lambda}{6}\hbar^2\frac{\delta^3 G}{\delta j^3}
\end{aligned}
$$

Отсюда

$$
m\left\{\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \omega_0^2\right\}\frac{\delta G}{\delta j} + \frac{\lambda}{6}\left(\frac{\delta G}{\delta j}\right)^3 - \frac{\lambda}{2}\mathrm{i}\hbar\frac{\delta G}{\delta j}\frac{\delta^2 G}{\delta j^2} - \frac{\lambda}{6}\hbar^2\frac{\delta^3 G}{\delta j^3} = j
$$

В этом случае уже не приходится говорить, что многоточечные функции Грина равны нулю, так как получающиеся уравнения существенно нелинейны и содержат вклады, зависящие от источника. Однако по-прежнему можно утверждать, что многоточечные функции не содержат вкладов, построенных в виде произведения одноточечных функций.

Вид уравнения Швингера-Дайсона для производящего функционала $G[j]$ на примере осциллятора показывает, что естественно определить квантовый аналог классической траектории как

$$
q_{\mathrm{cl}}(t) = \frac{\delta G[j]}{\delta j(t)}
$$

так что

$$
q_{\mathrm{cl}}(t)\big|_{j=0} = \left.\frac{\delta G[j]}{\delta j(t)}\right|_{j=0} = q_0(t)
$$

т. е. без источников в случае осциллятора получаем свободное движение, как это и должно быть, а при наличии, скажем, ангармоничности из 14.32 следует, что величина $q_{\mathrm{cl}}(t)$ удовлетворяет уравнению

$$
m\left\{\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \omega_0^2\right\}q_{\mathrm{cl}}(t) + \frac{\lambda}{6}q_{\mathrm{cl}}^3(t) - \frac{\lambda}{2}\mathrm{i}\hbar q_{\mathrm{cl}}(t)\frac{\delta q_{\mathrm{cl}}(t)}{\delta j} - \frac{\lambda}{6}\hbar^2\frac{\delta^2 q_{\mathrm{cl}}(t)}{\delta j^2} = j
$$

а значит, в пределе $\hbar \to 0$ получаем решение классического уравнения для $q(t)$ при наличии источников. Вклады с $\hbar$ приводят к квантовым поправкам. Преобразование Лежандра от j к q_{cl} приводит к функционалу

$$
\Gamma\left[q_{\mathrm{cl}}\right] = -\int q_{\mathrm{cl}}(t)j(t)\mathrm{d}t + G[j]
$$

который называют квантовым эффективным действием. Оно раскладывается в функциональный ряд по траекториям $\bar{q}_{\mathrm{cl}}(t) = q_{\mathrm{cl}}(t) - q_0(t)$ наподобие ряда для $G[j]$, причем по построению

$$
\frac{\delta\Gamma}{\delta q_{\mathrm{cl}}(t)} = -j(t)
$$

В разложении

$$\Gamma\left[q_{\mathrm{cl}}\right]=\Gamma^{(0)}+\int\Gamma^{(1)}(t)\bar{q}_{\mathrm{cl}}(t)\mathrm{d}t+\frac{1}{2!}\int\Gamma^{(2)}\left(t_1,t_2\right)\bar{q}_{\mathrm{cl}}\left(t_1\right)\bar{q}_{\mathrm{cl}}\left(t_2\right)\mathrm{d}t_1\ \mathrm{d}t_2+\ldots$$

коэффициентные функции называются многоточечными вершинами:

$$\Gamma^{(n)}=\Gamma_{(1\ldots n)}=\left.\frac{\delta^n\Gamma}{\delta q_{\mathrm{cl}}\left(t_1\right)\delta q_{\mathrm{cl}}\left(t_2\right)\ldots\delta q_{\mathrm{cl}}\left(t_n\right)}\right|_{q_{\mathrm{cl}}=q_0},$$

где мы ввели сокращенное обозначение для аргументов многоточечных функций. Поскольку при $j=0$ имеем $q_{\mathrm{cl}}(t)=q_0(t)$ или $\bar{q}_{\mathrm{cl}}=0$, замечаем, что разложение функционала Γ происходит также при нулевом значении источника j. Поэтому

$$\Gamma^{(1)}(t)=\left.\frac{\delta\Gamma}{\delta\bar{q}_{\mathrm{cl}}(t)}\right|_{\bar{q}_{\mathrm{cl}}=0}=\left.\frac{\delta\Gamma}{\delta\bar{q}_{\mathrm{cl}}(t)}\right|_{j=0}=-\left.j(t)\right|_{j=0}=0.$$

С учетом этих обозначений дифференцирование уравнения 14.34 при $t=t_1$ по $q_{\mathrm{cl}}\left(t_2\right)$ и условие $j=0$ дают

$$m\left\{\frac{\mathrm{d}^2}{\mathrm{d}t_1^2}+\omega_0^2\right\}\delta_{12}+\frac{\lambda}{2}q_0^2\left(t_1\right)\delta_{12}-\frac{\lambda}{2}\mathrm{i}\hbar\delta_{12}\mathcal{G}^{(2)}_{(11)}+$$
$$+\frac{\lambda}{2}\mathrm{i}\hbar q_0\left(t_1\right)\mathcal{G}^{(3)}_{(113)}\Gamma^{(2)}_{(32)}+\frac{\lambda}{6}\hbar^2\mathcal{G}^{(4)}_{(1113)}\Gamma^{(2)}_{(32)}=-\Gamma^{(2)}_{12},$$

где мы использовали равенство

$$\frac{\delta}{\delta q_{(2)}}=\frac{\delta j_{(3)}}{\delta q_{(2)}}\frac{\delta}{\delta j_{(3)}}=-\Gamma^{(2)}_{(32)}\frac{\delta}{\delta j_{(3)}}$$

и определения функций Грина. При этом, конечно,

$$\delta_{12}=\delta\left(t_1-t_2\right),\quad q_0\left(t_1\right)=\mathcal{G}^{(1)}\left(t_1\right)=\mathcal{G}^{(1)}_1$$

и мы использовали сокращенное обозначение для «свертки» индекса 3, например,

$$\mathcal{G}^{(3)}_{(113)}\Gamma^{(2)}_{(32)}=\int\mathcal{G}^{(3)}\left(t_1,t_1,t_3\right)\Gamma^{(2)}\left(t_3,t_2\right)\mathrm{d}t_3$$

Вариация второго порядка при нулевых источниках, очевидно, связана с обратной двухточечной функцией Грина:

$$\Gamma^{(2)}_{(12)}=\frac{\delta^2\Gamma}{\delta q_{\mathrm{cl}}\left(t_1\right)\delta q_{\mathrm{cl}}\left(t_2\right)}=-\frac{\delta j\left(t_1\right)}{\delta q_{\mathrm{cl}}\left(t_2\right)}=-\left[\frac{\delta q_{\mathrm{cl}}\left(t_2\right)}{\delta j\left(t_1\right)}\right]^{-1}=$$
$$=-\left[\frac{\delta^2 G}{\delta j\left(t_1\right)\delta j\left(t_2\right)}\right]^{-1}=-\left[\mathcal{G}^{(2)}_{(12)}\right]^{-1}$$

в смысле интегрального выражения

$$\Gamma^{(2)}_{(12)}\mathcal{G}^{(2)}_{(23)}=-\delta_{13}$$

Уравнение 14.37 справедливо не только при нулевом источнике, так что дифференцируя

$$\frac{\delta^2\Gamma}{\delta q_{(1)}\delta q_{(2)}}\frac{\delta^2 G}{\delta j_{(2)}\delta j_{(3)}}=-\delta_{13}$$

еще раз по $q_{\mathrm{cl}}\left(t_5\right)$, находим

$$\Gamma^{(3)}_{(12'5)}\mathcal{G}^{(2)}_{(2'3)} - \Gamma^{(2)}_{(12)}\mathcal{G}^{(3)}_{(234)}\Gamma^{(2)}_{(45)} = 0$$

или с учетом обратного двухточечного оператора

$$\Gamma^{(3)}_{(12'5)} = -\mathcal{G}^{(3)}_{(234)}\Gamma^{(2)}_{(12)}\Gamma^{(2)}_{(32')}\Gamma^{(2)}_{(45)} = \mathcal{G}^{(3)}_{(234)}\left[\mathcal{G}^{(2)}_{(12)}\right]^{-1}\left[\mathcal{G}^{(2)}_{(32')}\right]^{-1}\left[\mathcal{G}^{(2)}_{(45)}\right]^{-1}$$

и т. п. Поэтому говорят, что вершинные функции - усеченные функции Грина, т. е. функции внешние, исходящие из кружка, линии которых отсечены обратными двухточечными функциями Грина. При этом не все усеченные функции Грина дают вклад в вершинные функции, а только, как говорят, сильно связные (proper) или одночастично неприводимые (one-particle irreducible). Одночастично приводимые функции Грина соответствуют таким диаграммам, что на них найдётся хотя бы одна линия, при разрезании которой диаграмма становится несвязной. Этот факт мы докажем чуть ниже, а пока для примера, если пренебречь квантовыми поправками ($\hbar \to 0$) и взять третью производную уравнения (14.36 по q_{cl}, то получим вершину четвертой степени в эффективном действии Γ

$$\Gamma^{(4)}_{(1234)} \approx -\lambda\delta_{12}\delta_{13}\delta_{14}$$

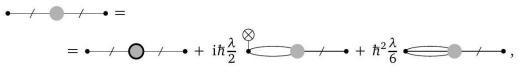
а соответствующая функция Грина

$$\mathcal{G}^{(4)}_{(1234)} \approx -\lambda\mathcal{G}^{(2)}_{(15)}\mathcal{G}^{(2)}_{(25)}\mathcal{G}^{(2)}_{(35)}\mathcal{G}^{(2)}_{(45)} + \ldots$$

С учетом сказанного уравнение для двухточечной вершиной функции 14.36 принимает вид

$$\Gamma^{(2)}_{(12)} = \left(-m\left\{\frac{\mathrm{d}^2}{\mathrm{d}t_1^2} + \omega_0^2\right\} - \frac{\lambda}{2}\left[\mathcal{G}^{(1)}_1\right]^2 + \frac{\lambda}{2}\mathrm{i}\hbar\mathcal{G}^{(2)}_{(11)}\right)\delta_{12} + \\ + \frac{\lambda}{2}\mathrm{i}\hbar\mathcal{G}^{1}_{(1)}\mathcal{G}^{(3)}_{(113)}\left[\mathcal{G}^{(2)}_{(32)}\right]^{-1} + \frac{\lambda}{6}\hbar^2\mathcal{G}^{(4)}_{(1113)}\left[\mathcal{G}^{(2)}_{(32)}\right]^{-1}$$

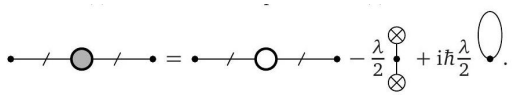
Это уравнение можно изобразить графически, если условиться обозначать вершинные функции так же, как и функции Грина, но с перечеркнутыми линиями. Итак,



где мы ввели обозначение

$$\left(-m\left\{\frac{\mathrm{d}^2}{\mathrm{d}t_1^2} + \omega_0^2\right\} - \frac{\lambda}{2}\left[\mathcal{G}^{(1)}_1\right]^2 + \frac{\lambda}{2}\mathrm{i}\hbar\mathcal{G}^{(2)}_{11}\right)\delta_{12} \longrightarrow \bullet, \bigcirc$$

Этот вклад можно также выразить в виде



Здесь же введена двухточечная вершинная функция для свободного осциллятора или, как говорят, собственная энергия осциллятора

$$-m\left\{\frac{\mathrm{d}^2}{\mathrm{d}t_1^2} + \omega_0^2\right\}\delta_{12} \longrightarrow \bullet, \bigcirc,$$

Напомним, что этот вклад-квадратичный член в квантовом эффективном действии, т. е. просто

$$\frac{1}{2}\Gamma_{(12)}q_{\rm cl}^{(1)}q_{\rm cl}^{(2)} = -\frac{m}{2}\int \mathrm{d}t\bar{q}_{\rm cl}(t)\left\{\frac{\mathrm{d}^2\bar{q}_{\rm cl}(t)}{\mathrm{d}t_1^2} + \omega_0^2\bar{q}_{\rm cl}(t)\right\} = \\ = \int \mathrm{d}t\left\{\frac{m}{2}\dot{\bar{q}}_{\rm cl}^2(t) - \frac{m\omega_0^2}{2}\bar{q}_{\rm cl}^2(t)\right\}$$

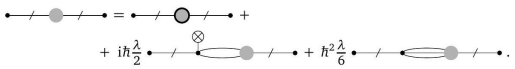
Подчеркнем, что каждая замкнутая петля приводит фактору ?.

Графическое представление уравнения Швингера-Дайсона

Графическое представление уравнения Швингера-Дайсона 14.38 для двухточечной вершинной функции становится еще более наглядным, если использовать тривиальное тождество

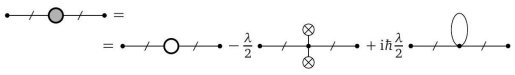
$$\left[\mathcal{G}^{(2)}_{1'4}\right]^{-1}\mathcal{G}^{(2)}_{41} = \delta_{11'}$$

Умножая уравнение на это тождество и интегрируя по $t_{1'}$, видим, что вклад с дельта-функцией не изменяется, а квантовые поправки теперь можно представить с использованием дополнительной усеченной двухточечной функции Грина («ампутированная нога»), так что



Эта запись «читается» так: двухточечная вершинная функция равна сумме вкладов собственной энергии с учетом квантовых эффектов самодействия и квантовых поправок за счет петель, причем однопетлевой вклад определяется трехточечной функцией Грина (кружок с тремя линиями) и «голой вершиной» q^4-взаимодействия λ (точка с четырьмя линиями), а двухпетлевой - «голой» четверной вершиной (точка с 4 линиями) и полной 4-точечной функцией Грина (кружок с 4 линиями).

Совершенно аналогично собственная энергия с квантовыми поправками представляется как



Значит, наряду с собственной энергией свободного осциллятора есть вклад от «голой» вершины λ с учетом граничных условий и однопетлевой вклад (так называемый «головастик»).

8.2.4 Strongly Connected Diagrams by Kiselev

(мб в КТП унесу, посмотрим, пока тут)

Теория

Докажем, что производящий функционал вершинных функций Γ содержит только сильно связные диаграммы. Для этого воспользуемся методом Сиднея Коулмена и Стивена Вайнберга: построим производящий функционал функций Грина не с исходным действием на траектории S, а с эффективным действием Γ,

$$Z_\Gamma[j] = \exp\left\{\frac{\mathrm{i}}{\hbar_\Gamma} G_\Gamma[j]\right\} = \mathcal{N}\int \mathcal{D}q \exp\left\{\frac{\mathrm{i}}{\hbar_\Gamma}\left(\Gamma + \int \mathrm{d}t q(t) j(t)\right)\right\}$$

где мы также провели формальную замену $\hbar \to \hbar_\Gamma$. Тогда $G_\Gamma[j]$ - это производящий функционал связных функций Грина с действием Γ. При этом, как мы установили, в пределе при $\hbar_\Gamma \to 0$ величина $G_\Gamma[j] \to G_\Gamma^{(0)}[j]$ не будет содержать петель, т. е. будет представлять собой, как говорят, лишь набор связных древесных диаграмм. Но в этом же пределе функциональный интеграл сводится к своему значению в стационарной точке:

$$\exp\left\{\frac{\mathrm{i}}{\hbar_\Gamma} G_\Gamma^{(0)}[j]\right\} = \lim_{\hbar_\Gamma \to 0} \int \mathcal{D}q \exp\left\{\frac{\mathrm{i}}{\hbar_\Gamma}\left(\Gamma + \int \mathrm{d}t q(t) j(t)\right)\right\} =$$
$$= \exp\left\{\frac{\mathrm{i}}{\hbar_\Gamma}\left(\Gamma + \int \mathrm{d}t q(t) j(t)\right)\right\}\Bigg|_{\delta\left[\Gamma + \int \mathrm{d}t q(t) j(t)\right]/\delta q(t) = 0}.$$

Условие стационарности означает, что

$$\frac{\delta\Gamma}{\delta q(t)} = -j(t), \quad G_\Gamma^{(0)} = \Gamma + \int q(t) j(t) \mathrm{d}t$$

т. е. предел производящего функционала в точности совпадает с производящим функционалом связных функций Грина в исходной теории:

$$G_\Gamma^{(0)} = G[j]$$

Таким образом, производящий функционал связных функций Грина соответствует связным древесным диаграммам с пропагаторами и вершинами, которые задаются эффективным действием Γ (см. рис. 23).

Важно, что остается справедливым соотношение

$$\Gamma^{(2)}_{(13)} \mathcal{G}^{(2)}_{(32)} = -\delta_{12}$$

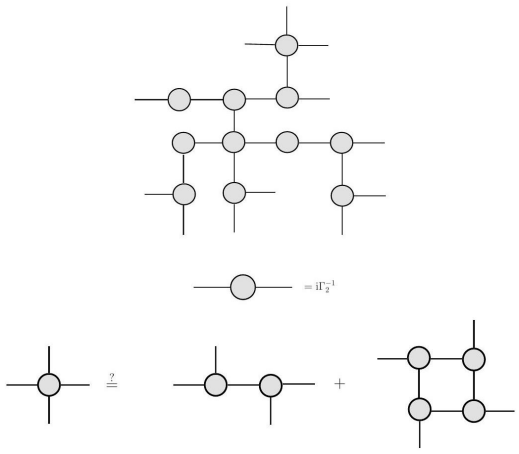


Рис. 23. Древесный предел $\hbar_\Gamma \to 0$ при построении G_Γ: пример дерева с многими ветвями, двухточечная функция Грина и 4 -точка Γ_4, представленная гипотетическим одночастично приводимым вкладом и петлей за счет 3-точечных вершин. Ясно, что одночастично приводимый вклад следует исключить по построению, поскольку он уже учтен при построении древесных диаграмм именно в качестве трехточечного сильно связного трехчастичного вклада.

так что связная двухточечная функция Грина $\mathcal{G}^{(2)}$ представляет собой двухточечную вершину $\Gamma^{(2)}$ с внешними линиями:

$$\mathrm{i}\mathcal{G}^{(2)}_{(12)} = \mathrm{i}\mathcal{G}^{(2)}_{(13)}\mathrm{i}\Gamma^{(2)}_{(33')}\mathrm{i}\mathcal{G}^{(2)}_{(3'2)}.$$

Более того, многократное повторение (вставка) блоков $\mathrm{i}\Gamma^{(2)}_{(33')}\mathrm{i}\mathcal{G}^{(2)}_{(3'2)}$ в эту диаграмму сводится к единичному оператору, т. е. все цепочки с многократной вставкой двухточечной вершины идентичны древесной диаграмме с одной двухточечной вершинной функцией!

Итак, связные функции Грина в $G[j]$ для исходной теории с затравочным действием S являются в то же время диаграммами, построенными в древесном приближении в теории, где затравочным является уже эффективное действие Г. Это значит, во-первых, что все такие древесные диаграммы, построенные по вершинам с эффективным действием, являются одночастично приводимыми: удаление любой внутренней линии делает диаграмму несвязной.

Во-вторых, никакая из вершин $\Gamma_{(1\ldots n)}$ в таких древесных диаграммах не может сама быть представлена как древесная, поскольку разложение такой вершины на сумму одночастично приводимых вкладов и одночастично неприводимый вклад означал бы, что вклад суммы одночастично приводимых диаграмм уже учтен прежде в виде такого же древесного вклада (см. илллюстрацию этого утверждения на примере 4-точки на рис. 23. Таким образом, по построению, если учтены все древесные вклады с одночастично неприводимыми вершинами низшего порядка, то вершины более высокого порядка уже не содержат одночастично приводимых вкладов.

Это можно доказать методом математической индукции. Сначала заметим, что все древесные вклады в $\mathcal{G}$, где есть вершина с одной внешней точкой $\Gamma^{(1)}$ равны нулю, так как $\delta\Gamma/\delta q_{\mathrm{cl}} = -j$ при $j = 0$ - это нуль. Потом рассмотрим все древесные диаграммы, где учтены все двухточечные вершины. Допустим, что двухточечная связная функция все же является одночастично приводимой. Тогда удаление в диаграмме внутренней линии делает диаграмму двусвязной, и у оставшихся двух компонент связности остаются два варианта по числу внешних линий: либо $2 + 0$ внешних линий, либо $1 + 1$ внешних линий. В первом варианте вторая компонента связности соединялась с диаграммой одной линией, т. е. она состояла из одноточечной функции, которую мы считаем равной нулю. Во втором варианте, обе компоненты связности до удаления внутренней линии были сформированы двухточечными функциями, а мы показали, что это сводится к одной двухточечной функции, и стало быть, такая диаграмма эквивалентна единственной двухточечной функции. Другими словами, в древесных диаграммах для построения связных функций Грина $\mathcal{G}$ из вершинных функций уже были учтены все двухточечные функции, и разбиение двухточечной вершины на древесную диаграмму из двух и более двухточечных вершин представляет собой тождественную операцию, которая ничего не меняет, и по этому двухточечную вершину можно считать сильно связной. Первый шаг индукции доказан.

Допустим теперь, что все вершинные функции с числом внешних точек меньше, чем n, являются сильно связными, а n-точечная вершинная функция имеет одночастично приводимый вклад. Это значит, что после разрезания внутренней линии в этом вкладе есть только два варианта для оставшихся компонент связности: в первом варианте у одной из компонент связности остается 0 внешних линий, и значит, эта компонента получилась из одночастичной вершины, которая равна нулю, и этот вариант невозможен. Во втором варианте, вклад в n-точечную вершинную функцию распадается на две вершинные функции, у каждой из которых число внешних точек до разрезания внутренней линии было меньше чем n, а значит, эти функции одночастично неприводимы согласно предположению о втором шаге индукции. Следовательно, одночастично приводимый вклад в n-точечную вершинную функцию построен как древесная диаграмма соединяющая две одночастично неприводимых функции. Но это

недопустимо, так как для связных функций Грина $\mathcal{G}$, построенных из вершинных функций Γ, уже учтены все древесные диаграммы с сильно связными вершинами с числом внешних точек меньше, чем n. Следовательно, и n-точечная вершинная функция может быть только одночастично неприводимой. Все шаги математической индукции выполнены.

Таким образом, доказано, что все вершинные функции должны быть одночастично неприводимыми (древесные вклады в вершины исключены, т.е. вершины либо голые, либо петли в терминах связных функций Грина для теории с исходным действием, причем, в особом случае двухточечной вершины надо иметь ввиду, что, как мы покажем, в качестве голой вершины выступает дважды усеченный, по числу внешних точек, древесный вклад.).

Покажем теперь, что вершинные функции - это усеченные сильносвязные функции Грина (одночастично неприводимые функции Грина с «ампутированными ногами»). В самом деле, рассмотрим

$$G[j] = \Gamma\left[q_{\mathrm{cl}}\right] - \int \mathrm{d}t q_{\mathrm{cl}}(t) \frac{\delta \Gamma}{\delta q_{\mathrm{cl}}(t)} = \Gamma\left[q_{\mathrm{cl}}\right] + \int \mathrm{d}t q_{\mathrm{cl}}(t) j(t)$$

Эффективное действие раскладывается в вариационный ряд

$$\Gamma\left[q_{\mathrm{cl}}\right] = \sum_{n'=0}^{\infty} \frac{1}{n'!} \Gamma_{(1' \ldots n')} q_{\mathrm{cl}}^{(1')} \ldots q_{\mathrm{cl}}^{(n')}$$

а само поле в вариационный ряд по внешнему току

$$\begin{aligned} q_{\mathrm{cl}}^{(k')} = \frac{\delta G}{\delta j_{(k')}} = \left.\frac{\delta G}{\delta j_{(k')}}\right|_{j=0} + \left.\frac{\delta^2 G}{\delta j_{(k')} \delta j_{(1)}}\right|_{j=0} j_{(1)} + \\ + \sum_{n=2}^{\infty} \frac{1}{n!} \left.\frac{\delta^{n+1} G}{\delta j_{(k')} \delta j_{(1)} \ldots j_{(n)}}\right|_{j=0} j_{(1)} \ldots j_{(n)} = \mathcal{G}^{(1)}\left(t_{k'}\right) + \mathcal{G}_{(k'1)} j_{(1)} + \\ + \sum_{n=2}^{\infty} \frac{1}{n!} \mathcal{G}_{(k'1 \ldots n)} j_{(1)} \ldots j_{(n)}, \end{aligned}$$

где для краткости изложения мы положим $\mathcal{G}^{(1)} = 0$, что легко сделать с помощью переопределения траектории координаты $\bar{q}_{\mathrm{cl}} \mapsto q_{\mathrm{cl}}$. Тогда переход в разложении эффективного потенциала от q_{cl} к источникам j в линейном приближении по токам дает вклад

$$\frac{1}{n!} \mathcal{G}'^{p}_{(1 \ldots n)} \prod_{k=1}^{n} j_{(k)} = \frac{1}{n!} \Gamma_{(1' \ldots n')} \prod_{k=1}^{n} \mathcal{G}_{(k'k)} j_{(k)}.$$

В этой формуле справа сильносвязные вершины $\Gamma_{(1' \ldots n')}$ домножаются по каждой своей внешней точке на двухточечную функцию Грина, а следовательно, в итоге и слева мы получаем сильносвязные диаграммы, которые мы пометили верхним индексом p (proper)! Это соотношение можно обратить и записать

$$\Gamma_{(1 \ldots n)} = \mathcal{G}'^{p}_{(1' \ldots n')} \prod_{k=1}^{n} \left(\mathcal{G}^{(2)}_{(kk')}\right)^{-1}$$

Это и означает, что вершины представляют собой связные одночастично неприводимые диаграммы для функций Грина $\mathcal{G}'^{p}_{(1 \ldots n)}$, в которых внешние линии ампутированы, т. е. пропагаторы этих линий удалены за счет домножения на обратный двухточечный связный пропагатор [1]

При рассмотрении нелинейного вклада в разложении $q_{\rm cl}$ по внешним токам 14.39) внешняя точка вершинной функции k' соединяется одной линией со связной функцией Грина $\mathcal{G}_{(k'1\ldots n)}, n \geqslant 2$, из которой исходят как минимум две линии во внешние точки функции Грина $\mathcal{G}$, но это значит, что нелинейные вклады отвечают одночастично приводимым диаграммам: именно разрезание этой единственной линии от точки k' вершины до связной диаграммы $\mathcal{G}_{(k'1\ldots n)}$ при $n \geqslant 2$ приводит к возникновению диаграммы с двумя компонентами связности.

Второе слагаемое в преобразовании Лежандра от вершин к связным функциям Грина

$$-\int \mathrm{d}t q_{\rm cl}(t)\frac{\delta\Gamma}{\delta q_{\rm cl}(t)}$$

устроено ровно также: квантовый аналог классической траектории $q_{\rm cl}$ также разлагается в вариационный ряд по внешнему току, а первая вариационная производная эффективного действия также может быть представлена как произведение сильносвязных вершин на полиномы по $q_{\rm cl}$, так что все рассуждения о связных функциях Грина и одночастично приводимых вкладах повторяются практически дословно. Различие возникает, если вариационную производную эффективного действия взять в линейном приближении по внешнему источнику, а «поле» $q_{\rm cl}$ разложить до членов порядка $n-1$. Тогда необходимо привести подобные члены.

Итак, единственное, что следует установить - это, как говорят, симметрийные факторы, которые задают коэффициент между одночастично неприводимыми функциями Грина $\mathcal{G}^p_{(1\ldots n)}$ и вершинами $\Gamma_{(1\ldots n)}$. Например, во втором порядке по внешним токам эффективное действие дает

$$\frac{1}{2}\Gamma_{(1'2')}\mathcal{G}_{(1'1)}\mathcal{G}_{(2'2)}j_{(1)}j_{(2)},$$

а второе слагаемое в преобразовании Лежандра, очевидно, как произведение двух линейных вкладов сводится к виду

$$-\Gamma_{(1'2')}\mathcal{G}_{(1'1)}\mathcal{G}_{(2'2)}j_{(1)}j_{(2)}$$

так что в сумме связная двухточечная функция Грина [2]

$$\mathcal{G}_{(12)} = -\Gamma_{(1'2')}\mathcal{G}_{(1'1)}\mathcal{G}_{(2'2)} = \delta_{12'}\mathcal{G}_{(2'2)} = \mathcal{G}_{(12)}$$

что и следовало ожидать. Симметрийный фактор здесь равен -1 (см. 14.42 в первом равестве).

[1] Штрих у символа $\mathcal{G}'^p_{(1\ldots n)}$ указывает на то, что мы рассмотрели не все вклады в одночастично неприводимые диаграммы.

[2] Напомним, что двухточечная вершина - обратная функция Грина со знаком минус! При $n > 2$ вклад эффективного действия

$$\frac{1}{n!}\Gamma_{(1'\ldots n')}\prod_{k=1}^{n}\mathcal{G}_{(k'k)}j_{(k)}$$

линейный член разложения поля по источнику при умножении на разложение первой вариационной производной Γ по источнику до членов порядка $n-1$ дает

$$-\mathcal{G}_{(1'1)}j_{(1)}\frac{1}{(n-1)!}\Gamma_{(1'\ldots n')}\prod_{k=2}^{n}\mathcal{G}_{(k'k)}j_{(k)}$$

а разложение поля по источнику до членов порядка $n-1$ при умножении на линейный член разложения первой вариационной производной Γ по источнику дает

$$-\frac{1}{(n-1)!}\mathcal{G}_{(1'2\ldots3)}\left(\prod_{k=2}^{n}j_{(k)}\right)\Gamma_{(1'1'')}\mathcal{G}_{(1''1)}j_{(1)}$$

Но, во-первых,

$$\Gamma_{(1'1'')}\mathcal{G}_{(1''1)}=-\delta_{1'1}$$

откуда

$$-\frac{1}{(n-1)!}\mathcal{G}_{(1'2\ldots3)}\left(\prod_{k=2}^{n}j_{(k)}\right)\Gamma_{(1'1'')}\mathcal{G}_{(1''1)}j_{(1)}=\frac{1}{(n-1)!}\mathcal{G}_{(12\ldots3)}\prod_{k=1}^{n}j_{(k)}.$$

Во-вторых, в этом слагаемом нас интересует только влад сильносвязных диаграмм, который задается формулой

$$\mathcal{G}^{p}_{(1\ldots n)}=\mathcal{C}\Gamma_{(1'\ldots n')}\prod_{k=1}^{n}\mathcal{G}^{(2)}_{(k'k)}$$

где $\mathcal{C}$ - искомый симметрийный фактор, для которого после учета всех слагаемых устанавливаем

$$\mathcal{C}=(1-n)+n\mathcal{C}\Rightarrow\mathcal{C}=1$$

Таким образом

$$\Gamma_{(1\ldots n)}=\mathcal{G}^{p}_{(1'\ldots n')}\prod_{k=1}^{n}\left(\mathcal{G}^{(2)}_{(kk')}\right)^{-1},\quad n>2$$

Если вариационные производные $Z[j]$ мы условились изображать в виде линий, исходящих из овала, а овал можно затем представить в виде сумм диаграмм в теории возмущений с распространением частиц вдоль тех же линий, то в той же логике можно условиться изображать вариационные производные $G[j]$ в виде линий, исходящих из круга, где круг можно затем представить в виде сумм связных диаграмм с вершинами в теории возмущений и с распространением частиц вдоль линий, пересекающихся в вершинах. Тогда принято изображать вариационные производные эффективного действия Γ

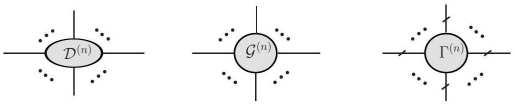


Рис. 24. Вариационные производные для амплитуды $Z[j]$, производящего функционала связных функций $G[j]$ и вершины $\Gamma\left(q_{\mathrm{cl}}\right)$, соответственно.

в виде круга с исходящими из него перечеркнутыми линиями, которые символизируют усеченные внешние пропагаторы («ампутированные ноги»), как это показано на рис. 24

Наконец, укажем альтернативный способ построения теории возмущений в терминах континуального интеграла и, следовательно, диаграмм Фейнмана в теории возмущений. Пусть гамильтониан представлен в виде

$$\mathcal{H}=\frac{p^2}{2m}+\frac{m\omega_0^2}{2}q^2+V_{\mathrm{int}}\left(q\right)-j(t)q$$

где V_{int} - малое возмущение. Тогда производящий функционал

$$Z[j] = \mathcal{N} \int \mathcal{D}q \exp\left\{ \frac{\mathrm{i}}{\hbar} \int\limits_{t'}^{t''} \mathrm{d}t \left[\frac{m\dot{q}^2(t)}{2} - \frac{m\omega_0^2}{2} q^2(t) - V_{\mathrm{int}}(q(t)) + j(t)q(t) \right] \right\}$$

можно переписать в виде

$$Z[j] = \mathcal{N} \exp\left\{ -\frac{\mathrm{i}}{\hbar} \int\limits_{t'}^{t''} \mathrm{d}t V_{\mathrm{int}} \left(-\mathrm{i}\hbar \frac{\delta}{\delta j(t)} \right) \right\} \times$$

$$\times \int \mathcal{D}q \exp\left\{ \frac{\mathrm{i}}{\hbar} \int\limits_{t'}^{t''} \mathrm{d}t \left[\frac{m\dot{q}^2(t)}{2} - \frac{m\omega_0^2}{2} q^2(t) + j(t)q(t) \right] \right\},$$

где мы воспользовались тем, что значение координаты на траектории под знаком интегрирования получается при вариации континуального интеграла. Значит, производящий функционал при наличии возмущения выражается через действие дифференциального оператора на производящий функционал для свободного осциллятора:

$$Z[j] = \exp\left\{ -\frac{\mathrm{i}}{\hbar} \int\limits_{t'}^{t''} \mathrm{d}t V_{\mathrm{int}} \left(-\mathrm{i}\hbar \frac{\delta}{\delta j(t)} \right) \right\} Z_{\mathrm{osc}}[j]$$

где, как мы выяснили,

$$Z_{\mathrm{osc}}[j] = \mathrm{e}^{\frac{\mathrm{i}}{\hbar} G[j]}$$

$$G[j] = \mathcal{G}_0 + \int \mathcal{G}^{(1)}(t) j(t) \mathrm{d}t + \frac{1}{2!} \int \mathcal{G}^{(2)}\left(t_1, t_2\right) j\left(t_1\right) j\left(t_2\right) \mathrm{d}t_1 \, \mathrm{d}t_2.$$

Дальнейшая процедура построения правил Фейнмана для многоточечных функций Грина задается вариационным дифференцированием в последовательном порядке малости по возмущению. Мы не будем рассматривать здесь далее этот вариант построения теорий возмущений в рамках интеграла по траекториям, поскольку это обычно относят к курсу квантовой теории поля.

Укажем однако, что формула 14.44 позволяет найти общее соотношение для числа петель, степени возмущения и числа внутренних линий в связной диаграмме. Действительно, если N_V - степень вклада возмущения в функцию Грина, то это значит, что N_V - это число внутренних вершин в диаграмме N_V (vertex, number of vertecies). Если в диаграмме есть внутренняя линия, то она соединяет 2 точки между вершинами, так что при последовательном счете, если рассматривать связную цепочку из N_I внутренних линий (internal lines), в этой цепочке имеется $N_I + 1$ вершин как сумма вершин на конце внутренней линии плюс одна вершина в начале цепочки внутренних линий. Однако на связной диаграмме некоторые конечные точки в цепочке внутренних линий могут совпасть с начальными точками внутренних линий. Каждое такое совпадение означает наличие замкнутой петли. Число петель N_L (loop, number of loops) определяет число точек посчитанных дважды, так что общее число вершин на связной диаграмме (напомним, у связной диаграммы только одна компонента связности, т. е. одна непрерывная цепочка внутренних линий, на которой возможны ветвления и пересечения) в действительности равно

$$N_V = N_I + 1 - N_L, \quad N_L = N_I + 1 - N_V.$$

В справедливости данной формулы читатель может наглядно убедиться на примере четырех- и двухточечной функции Грина в теории «фи-в-четвертой», как это показано на рис. 25.

Рис. 25. Диаграммы с одной и двумя вершинами в модели $V[\phi] \sim \lambda\phi^4$ с разным числом внутренних линий (слева направо): 0, 1, 3, - и петель:0, 1, 2.

Заметим теперь, что связные функции Грина $\mathrm{i}G[j]/\hbar$ с фиксированным числом петель получаются суммированием диаграмм с N_V степенями возмущения и N_I внутренними линиями, причем каждое возмущение дает фактор $1/\hbar$, а каждая внутренняя линия отвечает обратному оператору на квадратичном по траектории свободном действии, т. е. вносит фактор $\hbar$ (см. связь связной двухточечной функции Грина со связной частью двухточечной функции Грина для амплитуды вероятности $Z[j]$). В итоге связные функции Грина с петлями имеют следующий масштаб по $\hbar$:

$$\text{scale } \frac{1}{\hbar}G^{(L)} \sim \text{ scale } \sum_{N_V,N_I} \left(\frac{1}{\hbar}\right)^{N_V} \hbar^{N_I}\Bigg|_{N_L \text{ fixed}} \sim \text{ scale } \hbar^{N_L-1}.$$

Таким образом, разложение связных функций Грина по петлям совпадает с разложением по степеням $\hbar$! Это означает, что в классическом пределе $\hbar \to 0$ среди связных диаграмм остаются только диаграммы без петель или, как говорят, древесные диаграммы.

Подчеркнем также, что полученные выше закономерности, связанные с числом петель, никак не зависят от того, как устроено возмущение (кубическое по полям или высшей степени по полям) и сколько внешних линий имеют связные функции Грина.

Итак, наряду с решением задачи вычисления амплитуд квантовых переходов при наличии произвольного внешнего источника, фейнмановский интеграл по траекториям позволяет, во-первых, эффективно строить теорию возмущений при введении малой добавки к потенциалу. Во-вторых, по своему определению он дает метод численного интегрирования квантовых задач, не поддающихся анализу в рамках теории возмущений. В-третьих, континуальный интеграл в квантовой теории поля позволяет наиболее наглядно и просто получать соотношения между функциями Грина при наличии симметрий исходного классического действия и выявлять квантовые аномалии, т. е. случаи принципиально непреодолимого нарушения симметрии классического действия при квантовании, и т. п.

8.2.5 $\mathcal{S}-$Matrix Functional

(мб в КТП унесу, посмотрим, пока тут)

Теория

Для граничных условий в голоморфном представлении введем решение классического уравнения движения для свободного осциллятора [1]

$$q_0(t) = x_0\left(\alpha_{\text{in}}\,\mathrm{e}^{-\mathrm{i}\omega_0 t} + \bar{\alpha}_{\text{out}}\,\mathrm{e}^{\mathrm{i}\omega_0 t}\right), \quad x_0 = \sqrt{\frac{\hbar}{2m\omega_0}}$$

и рассмотрим голоморфное ядро $\mathcal{S}$-матрицы как функционал от этого решения, т. е. запишем его в виде

$$\mathcal{S}\left(\bar{\alpha}_{\text{out}}\,,\alpha_{\text{in}}\right)\cong\mathcal{S}\left[q_0(t)\right]=\exp\left\{-\frac{\mathrm{i}}{\hbar}\int\limits_{t'}^{t''}\mathrm{d}tV_{\text{int}}\,\left(-\mathrm{i}\hbar\frac{\delta}{\delta j(t)}\right)\right\}Z_{\text{osc}}\left[j\right]\Bigg|_{j=0}$$

где

$$Z_{\text{osc}}\left[j\right]=\exp\left\{\int\mathcal{G}^{(1)}(t)j(t)\mathrm{d}t+\frac{1}{2!}\int\mathcal{G}^{(2)}\left(t_1-t_2\right)j\left(t_1\right)j\left(t_2\right)\mathrm{d}t_1\,\mathrm{d}t_2\right\}$$

[1] Выражение $\sqrt{14.45}$, конечно, является решением однородного линейного уравнения для свободных колебаний, но оно, вообще говоря, комплекснозначное, так что трактовать его следует как матричный элемент координаты по когерентным состояниям в начале и в конце эволюции, который домножен на такой нормировочный фактор, который приводит к формуле 14.45.

$$\mathcal{G}^{(1)}(t)=q_0(t)$$

Разложение этого функционала в ряд

$$\mathcal{S}\left[q_0(t)\right]=\sum_{n=1}^{\infty}\frac{(-\mathrm{i}\hbar)^n}{n!}\mathcal{S}^{(n)}\left(t_1,...,t_n\right)\prod_{k=1}^{n}q_0\left(t_k\right)\mathrm{d}t_k$$

имеет наглядный физический смысл: коэффициентные функции $\mathcal{S}^{(n)}$ задают амплитуды перехода одного асимптотического состояния в другое с общей суммой квантов в исходном и конечном состояниях, равной n. В самом деле, дифференцирование по параметру начального состояния α_{in} и конечного $\bar{\alpha}_{\text{out}}$ можно представить как вариационную производную

$$\frac{\partial^{m+n}\mathcal{S}[q_0]}{\partial\alpha_{\text{in}}^m\partial\bar{\alpha}_{\text{out}}^n}\Bigg|_{\alpha_{\text{in}}=\bar{\alpha}_{\text{out}}=0}=\int\frac{\delta^{m+n}\mathcal{S}[q_0]}{\delta q_0(t_1)...\delta q_0(t_{m+n})}\Bigg|_{q_0=0}\times\\ \times\prod_{k=1}^{m}\frac{\partial q_0(t_k)}{\partial\alpha_{\text{in}}}\mathrm{d}t_k\prod_{l=1}^{n}\frac{\partial q_0(t_l)}{\partial\bar{\alpha}_{\text{out}}}\mathrm{d}t_l,$$

где

$$\frac{\partial q_0(t)}{\partial\bar{\alpha}_{\text{out}}}=x_0\mathrm{e}^{\mathrm{i}\omega_0 t},\quad\frac{\partial q_0(t)}{\partial\alpha_{\text{in}}}=x_0\mathrm{e}^{-\mathrm{i}\omega_0 t}$$

так что в правой части 14.49 стоит фурье-образ коэффициентной функции

$$\int\mathcal{S}^{(m+n)}\left(t_1,...,t_{m+n}\right)\prod_{k=1}^{m}\mathrm{e}^{-\mathrm{i}\omega_0 t_k}\,\mathrm{d}t_k\prod_{l=1}^{n}\mathrm{e}^{\mathrm{i}\omega_0 t_l}\,\mathrm{d}t_l=\\ =\tilde{\mathcal{S}}^{(m+n)}(\underbrace{\omega_0,...,\omega_0}_{m},\underbrace{-\omega_0,...,-\omega_0}_{n}).$$

С левой же стороны 14.49 согласно 13.65 стоит производная от голоморфного ядра оператора эволюции при нулевых источниках, т. е.

$$\frac{\partial^{m+n}\mathcal{S}\left[q_0\right]}{\partial\alpha_{\text{in}}^m\partial\bar{\alpha}_{\text{out}}^n}\Bigg|_{\alpha_{\text{in}}=\bar{\alpha}_{\text{out}}=0}=\sqrt{n!m!\mathcal{S}_{nm}}.$$

При этом матричный элемент

$$\mathcal{S}_{nm}=\left\langle n\left|\hat{U}\left(t'',t'\right)\right|m\right\rangle,\quad t''\to+\infty,\quad t'\to-\infty$$

и есть амплитуда перехода в ходе эволюции из начального состояния с m квантами в конечное состояние с n квантами 1

Редукиионные формуль. Найдем теперь связь между амплитудами переходов $\mathcal{S}^{(n)}$ и функциями Грина $\mathcal{D}^{(n)}$. Для этого заметим, что

$$\int \mathcal{G}^{(1)}(t)j(t)\mathrm{d}t + \frac{1}{2!}\int \mathcal{G}^{(2)}\left(t_1,t_2\right)j\left(t_1\right)j\left(t_2\right)\mathrm{d}t_1\ \mathrm{d}t_2 = \\ = \frac{1}{2!}\int \mathcal{G}^{(2)}\left(t_1,t_2\right)\tilde{j}\left(t_1\right)\tilde{j}\left(t_2\right)\mathrm{d}t_1\ \mathrm{d}t_2$$

1 В действительности многие подобные амплитуды могут оказаться равными нулю в силу законов сохранения энергии и т. п. где

$$\tilde{j}(t) = j(t) + \int \left[\mathcal{G}^{(2)}(t,\tilde{t})\right]^{-1}\mathcal{G}^{(1)}(\tilde{t})\mathrm{d}\tilde{t}$$

причем возникающий дополнительно вклад

$$\int \left[\mathcal{G}^{(2)}(t,\tilde{t})\right]^{-1}\mathcal{G}^{(1)}(\tilde{t})\mathcal{G}^{(1)}(t)\mathrm{d}\tilde{t}\ \mathrm{d}t = 0$$

так как $\mathcal{G}^{(1)}(t) = q_0(t)$ - решение уравнения свободного движения осциллятор[1]

Поэтому вариация функционала $\mathcal{S}$-матрицы согласно 14.46 сводится к вариации производящего функционала функций Грина $Z[\tilde{j}]$

$$-\mathrm{i}\hbar\frac{\delta\mathcal{S}\left[q_0\right]}{\delta q_0(t)}\bigg|_{j=0} = -\mathrm{i}\hbar\int\frac{\delta Z[\tilde{j}]}{\delta\tilde{j}(\tilde{t})}\frac{\delta\tilde{j}(\tilde{t})}{\delta q_0(t)}\mathrm{d}\tilde{t}\bigg|_{\tilde{j}=0}.$$

Но так как

$$\frac{\delta\tilde{j}(\tilde{t})}{\delta q_0(t)} = \left[\mathcal{G}^{(2)}(t,\tilde{t})\right]^{-1} = m\left\{\frac{\mathrm{d}^2}{\mathrm{d}t^2}+\omega_0^2\right\}\delta(t-\tilde{t})$$

интегрирование «снимается», и

$$\frac{\delta\mathcal{S}\left[q_0\right]}{\delta q_0(t)}\bigg|_{j=0} = m\left\{\frac{\mathrm{d}^2}{\mathrm{d}t^2}+\omega_0^2\right\}\frac{\delta Z[\tilde{j}]}{\delta\tilde{j}(t)}\bigg|_{\tilde{j}=0}$$

а значит,

$$\mathcal{S}^{(n)}\left(t_1,...,t_n\right) = \left(\prod_{k=1}^{n} m\left\{\frac{\mathrm{d}^2}{\mathrm{d}t_k^2}+\omega_0^2\right\}\right)\mathcal{D}^{(n)}\left(t_1,...,t_n\right)$$

Это и есть редукционные формулы: матричные элементы $\mathcal{S}$-матрицы получаются из функций Грина для производящего функционала оператора эволюции $\mathcal{D}$ усечением каждой линии фактором обратной связной двухточечной функции Грина для свободного осциллятора Если графически представить функции $\mathcal{D}$ аналогично функциям Грина $\mathcal{G}$, заменив кружок на овал для двухточечной функции

$$\mathcal{D}^{(2)} = \longrightarrow$$

а усечение внешних линий свободным пропагатором осциллятора двойным перечеркиванием, то, к примеру,

$$\mathcal{S}^{(2)} = \leftrightarrow \mathbb{H} \longrightarrow$$

При этом, конечно, нужно помнить о том, что многоточечные функции $\mathcal{D}$ построены из связных функций $\mathcal{G}$ и поэтому включают в себя несвязные диаграммы.

Нормалъный символ. Наряду с голоморфным ядром оператора $\hat{A}$ часто рассматривают и его нормальный символ, определенный разложением

[1] В других вкладах необходимо аккуратно обращаться с произведением двухточечной функции Грина на обратную к ней. оператора в ряд по нормально упорядоченным произведениям операторов рождения и уничтожения:

$$\hat{A} = \sum_{n,m} \mathcal{A}^N_{nm} \frac{\left(\hat{a}^\dagger\right)^n}{\sqrt{n!}} \frac{\hat{a}^m}{\sqrt{m!}}$$

где коэффициенты разложения $\mathcal{A}^N_{nm}$, конечно, не совпадают с матричными элементами оператора. Матричный элемент по когерентным состояниям -

$$\left\langle \alpha_{\rm out} \left| \hat{A} \right| \alpha_{\rm in} \right\rangle = \sum_{n,m} \mathcal{A}^N_{nm} \frac{\bar{\alpha}^n_{\rm out}}{\sqrt{n!}} \frac{\alpha^m_{\rm in}}{\sqrt{m!}} \left\langle \alpha_{\rm out} \left| \alpha_{\rm in} \right. \right\rangle .$$

Величину

$$\mathcal{A}^N \left(\bar{\alpha}_{\rm out} , \alpha_{\rm in} \right) = \sum_{n,m} \mathcal{A}^N_{nm} \frac{\bar{\alpha}^n_{\rm out}}{\sqrt{n!}} \frac{\alpha^m_{\rm in}}{\sqrt{m!}}$$

называют голоморфным ядром нормального символа оператора 1. Тогда из

$$\left\langle \alpha_{\rm out} \left| \alpha_{\rm in} \right. \right\rangle = \exp\left\{ -\frac{\bar{\alpha}_{\rm out}\, \alpha_{\rm out}}{2} - \frac{\bar{\alpha}_{\rm in}\, \alpha_{\rm in}}{2} + \bar{\alpha}_{\rm out}\, \alpha_{\rm in} \right\}$$

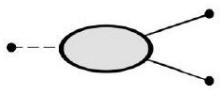
и определения ядра оператора следует связь

$$\mathcal{A}\left(\bar{\alpha}_{\rm out} , \alpha_{\rm in} \right) = \mathrm{e}^{\bar{\alpha}_{\rm out}\, \alpha_{\rm in}}\, \mathcal{A}^N \left(\bar{\alpha}_{\rm out} , \alpha_{\rm in} \right)$$

которая устанавливает соотношение между голоморфным ядром оператора и ядром его нормального символа. В литературе, использующей голоморфные представления, часто цитируется эта формула (развитие формализма континуального интеграла в квантовой механике и теории поля см. в учебном пособии 23).

Фермионный осциляятор. Построенное нами ранее голоморфное представление для фермионного осциллятора позволяет повторить для него процедуру введения интеграла по траекториям с той лишь разницей, что интегрирование ведется по грассмановым переменным.

Взаимодействие осциляяторов. Рассмотрим пример. Допустим, что физическая система включает в себя два различных осциллятора: обобщенные координаты - q_1 и q_2, частоты свободных колебаний $-\omega_1$ и ω_2. Если мы знаем, что $\omega_1 = 2\omega_2$ и при этом условии квант первого осциллятора может переходить в пару квантов второго осциллятора (сохранение энергии) с амплитудой λ, то как выглядит потенциал взаимодействия этих осцилляторов? Очевидно, что описанный процесс распада кванта первого осциллятора (штриховая линия) на пару квантов второго (сплошные линии) соответствует диаграмме



,

которая показывает уничтожение кванта типа 1 и рождение двух квантов типа 2. Эту амплитуду можно записать как

$$\left\langle 2'' \left| \hat{U} \right| 1' \right\rangle = \mathrm{i}\lambda$$

[1] Голоморфность является явной по построению. или в рамках теории возмущений

$$\mathrm{i}\lambda \longrightarrow \langle 0|\hat{a}_2\left(t''\right)\hat{a}_2\left(t''\right)\hat{U}\left(t'',t'\right)\hat{a}_1^\dagger\left(t'\right)|0\rangle =$$
$$= \left\langle 0\left|\hat{a}_2\left(t''\right)\hat{a}_2\left(t''\right)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int \mathrm{d}t\hat{H}_{\mathrm{int}}}\hat{a}_1^\dagger\left(t'\right)\right|0\right\rangle \approx$$
$$\approx \left\langle 0\left|\hat{a}_2\left(t''\right)\hat{a}_2\left(t''\right)\left\{1-\frac{\mathrm{i}}{\hbar}\int\limits_{t'}^{t''}\mathrm{d}t(-1)\hbar\lambda\hat{a}_2^\dagger(t)\hat{a}_2^\dagger(t)\hat{a}_1(t)\right\}\hat{a}_1^\dagger\left(t'\right)\right|0\right\rangle.$$

Но это есть не что иное, как амплитуда перехода, которая возникает при введении взаимодействия

$$V_{\mathrm{int}} = -\hbar\lambda\hat{a}_2^\dagger\hat{a}_2^\dagger\hat{a}_1 + \text{ h.c.},$$

где мы добавили эрмитово сопряженный вклад для вещественности потенциала и не приводим зависимость операторов от времени. Постоянная взаимодействия λ, очевидно, должна иметь размерность частоты. Значит,

$$V_{\mathrm{int}} \sim -\lambda\sqrt{\frac{8m_1m_2^2\omega_1\omega_2^2}{\hbar}}q_1q_2^2 \sim V_0\frac{q_1q_2^2}{\ell^3}$$

где мы учли связь операторов рождения и уничтожения с динамической переменной, а также ввели параметр энергии $V_0 = -\lambda\hbar$ и длину $\ell = \left(\hbar^3/8m_1m_2^2\omega_1\omega_2^2\right)^{1/6}$.

Таким образом, эмпирические наблюдения, т. е. измерения эффективного квантового действия, позволяют в рамках теории возмущений вводить члены с взаимодействием квантовых систем.

8.3 Scattering Theory: Features, Specific Models

8.3.1 1D delta-potential

(here will be basic theory)

8.3.2 Regularization methods for delta-function potential in two-dimensional quantum mechanics by Su-Long Nyeo

(see his article in Google for now)

8.3.3 2D scattering theory

2D Green's function

(??? приведу ее вывод. пока не додумал еще)

Developing 2D scattering theory based on a partial-wave analysis for an axially-symmetric potential $U(\rho)$ by GKKG.13.23

A theory of scattering for an axially-symmetric potential in two dimensions can be developed along the same lines as that for a spherically-symmetric potential in three dimensional quantum mechanics.

The Hamiltonian in an axially-symmetric field has the form:

$$\hat{H} = -\frac{\hbar^2}{2\mu}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right) + U(\rho) \tag{1}$$

while the solution of the Schrdinger equation has the following asymptotic behavior

$$\psi_{\mathbf{k}}^{+}(\boldsymbol{\rho}) \approx e^{ik\rho\cos\varphi} + \sqrt{i}\frac{f(k,\varphi)}{\sqrt{\rho}}e^{ik\rho}, \quad \rho \to \infty \tag{2}$$

Incident particles move in the direction of the positive x axis; here, $x = \rho\cos\varphi$. Note that now the scattered wave is cylindrical (not spherical), and so instead of $1/r$ we have $1/\sqrt{\rho}$. In this two-dimensional case, the scattering amplitude, $f(k,\varphi)$, has the physical dimension of the square root of length, and the physical dimension of the differential scattering cross-section $d\sigma/d\varphi = |f|^2$ is length. Finally, a phase factor $\sqrt{i}$ is used for convenience.

Since the operator $\hat{l}_z = -i\partial/\partial\varphi$ commutes with both the Hamiltonian of free motion and Hamiltonian (1), then the two-dimensional plane wave and the exact wavefunction $\psi_{\mathbf{k}}^{+}(\boldsymbol{\rho})$ can be expanded in the eigenfunctions, $\psi_m = e^{im\varphi}$, of this operator (analogous to the expansion over spherical functions in the case of a central potential):

$$e^{ik\rho\cos\varphi} = \sum_{m=-\infty}^{\infty} A_m J_{|m|}(k\rho)e^{im\varphi}, \quad \psi_{\mathbf{k}}^{+} = \sum_{m=-\infty}^{\infty} B_m R_{km}(\rho)e^{im\varphi} \tag{3}$$

Here, we have taken into account that the radial function of free motion with an "angular momentum" m is expressed in terms of the Bessel functions $J_{|m|}(k\rho)$, with the coefficients $A_m = i^{|m|}$. The values of the coefficients B_m are determined from the condition that the difference, $\psi_{\mathbf{k}}^{+} - e^{ikx}$, at large distances contains the outgoing waves, $\propto e^{ik\rho}$, for each term of the sum over m. Writing the asymptote of the radial function in the form [329]

$$R_{km}(\rho) = \sqrt{\frac{2}{\pi k\rho}}\sin\left(k\rho - \frac{\pi|m|}{2} + \frac{\pi}{4} + \delta_m\right) \tag{4}$$

we find $B_m = e^{i\delta_m}A_m$. As a result, we obtain a partial-wave decomposition of the scattering amplitude:

[329] The normalization factor in this function and the phase δ_m are chosen so that for $\delta_m = 0$, asymptote (4) coincides with the asymptote of a Bessel function, which describes the radial function of free motion.

$$f(k,\varphi) = \frac{1}{i\sqrt{2\pi k}}\sum_{m=-\infty}^{\infty}\left(e^{2i\delta_m} - 1\right)e^{im\varphi} \tag{5}$$

Note that the phase shift δ_m does not depend on the sign of m.
According to Eq. (5), the total scattering cross-section is

$$\sigma = \int_0^{2\pi}|f|^2 d\varphi = \frac{4}{k}\sum_{m=-\infty}^{\infty}\sin^2\delta_m \tag{6}$$

and the optical theorem in this two-dimensional case reads

$$\mathrm{Im}\, f(k,\varphi=0) = \sqrt{\frac{k}{8\pi}}\sigma(E) \tag{7}$$

Notice that extracting the factor $\sqrt{i}$ in Eq. (2) in the Born approximation is indeed convenient, as this convention ensures that for $|\delta_m| \ll 1$, the scattering amplitude given becomes real, according to Eq. (5).

Как в формулах для 3D рассеяния учесть ограниченность пространства и получить формулы 2D?

(??? вопрос на более глубокое понимание, пока не знаю и вряд ли скоро буду про это думать.)

Examples of 2D scatterings

2D scattering on δ-potential

Используем импульсное представление,

$$\frac{p^2}{2m}\psi(\boldsymbol{p}) + U_p \int (d\boldsymbol{p}')\,\psi(\boldsymbol{p}') = E\psi(\boldsymbol{p})$$

$$\psi(\boldsymbol{p}) = -\frac{U_{\boldsymbol{p}}}{-E + \frac{p^2}{2m}} \int (d\boldsymbol{p}')\,\psi(\boldsymbol{p}')$$

В размерности $d = 2$ интеграл расходится логарифмически на малых и на больших импульсах.

На больших импульсах очевидным образом интеграл нужно обрезать на масштабах $\sim 1/a$, поскольку это уравнение было выведено именно в таком предположении (это позволило нам заменить U_p на $U_{p=0}$; и поскольку интеграл логарифмический, то он нечувствителен к этой обрезке - она меняет лишь константу под логарифмом), а на маленьких - масштабом $\sqrt{2mE}$; сингулярность на малых энергиях оказывается слабой, логарифмической.

Поэтому чтобы сделать левую часть порядка единицы, уровень энергии иу очежо малежъким.

Приступим теперь к непосредственному вычислению:

$$\int \frac{d^2\boldsymbol{p}}{(2\pi)^2}\frac{1}{|E| + \frac{p^2}{2m}} = \int \frac{2\pi p dp}{4\pi^2}\frac{1}{|E| + \frac{p^2}{2m}} \approx \frac{m}{\pi}\int\limits_{\sim\sqrt{mE}}^{\sim 1/a} \frac{dp}{p} = \frac{m}{2\pi}\ln\frac{\#}{ma^2|E|}$$

Точность этого выражения следующая: число перед логарифмом определено точно, а в силу неточности при обрезании, число под логарифмом неизвестно.

Для его нахождения нужно решать уравнение Шрёдингера точно; это число уже определяется явным видом потенциала.

Тем самым, решая уравнение самосогласования, мы получаем (восстанавливая опять $\hbar$ по размерности) :

$$|E| = \#\frac{\hbar^2}{ma^2}\exp\left(-\frac{2\pi\hbar^2}{m}\left|\int U(\boldsymbol{r})d^2\boldsymbol{r}\right|^{-1}\right)$$

Таким образом, мы определили уровень энергии в мелкой двумерной яме с экспоненциальной точностью; и этот уро-оказывается действительно экспоненциально мелким.

Ведущая асимптотика даётся этой самой экспонентой, которая может быть оценена как $\exp\left(-\frac{\hbar^2/ma^2}{II_C}\right) \lll 1$. Число же в предэкспоненте таким способом определить нельзя.

Заметим, что в Левитове Шитове какой-то полнейший бред написан про эту задачу! Хотя, может, есть и другой способ обрезать интеграл тут...

2D delta-potential

8.3.4 Formalism of 3D Scattering Theory by Takhtajan

Здесь мы обрисуем теорию рассеяния для оператора Шрёдингера $H = -\Delta + V(\boldsymbol{x})$ (где мы положим $\hbar = 1$ и $\mu = \frac{1}{2}$) с быстро убывающим потенциалом. Конкретно, предположим, что ограниченная вещественнозначная функция $V(\boldsymbol{x})$ на $\mathbb{R}^3$ удовлетворяет условию

$$V(x) = O\left(|x|^{-3-\varepsilon}\right) \quad \text{при} \quad |x| \to \infty$$

для некоторого $\varepsilon > 0$. Тогда для любого $k \in \mathbb{R}^3$ уравнение Шрёдингера

$$-\Delta\psi(\boldsymbol{x}) + V(\boldsymbol{x})\psi(\boldsymbol{x}) = k^2\psi(\boldsymbol{x}), \quad k = |\boldsymbol{k}|,$$

имеет два решения $u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})$, удовлетворяющих следующим асимптотическим условиям при $|\boldsymbol{x}| \to \infty$:

$$u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k}) = e^{i\boldsymbol{k}\boldsymbol{x}} + f^{(\pm)}(k, \boldsymbol{\omega}, \boldsymbol{n})\frac{e^{\pm ikr}}{r} + o\left(\frac{1}{r}\right),$$

где $\boldsymbol{k} = k\boldsymbol{\omega}, \boldsymbol{x} = r\boldsymbol{n}$. Асимптотики (4.7) называются условиями излучения Зоммерфельда. Для доказательства существования решений $u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})$ надо рассмотреть следующие интегральные уравнения:

$$u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k}) = e^{i\boldsymbol{k}\boldsymbol{x}} + \int\limits_{\mathbb{R}^3} G^{(\pm)}(\boldsymbol{x} - \boldsymbol{y}, k)V(\boldsymbol{y})u^{(\pm)}(\boldsymbol{y}, \boldsymbol{k})d^3\boldsymbol{y}$$

где

$$G^{(\pm)}(\boldsymbol{x}, k) = -\frac{1}{4\pi}\frac{e^{\pm ikr}}{r}$$

Интегральные уравнения (4.8) эквивалентны уравнению Шрёдингера (4.6) с условиями излучения Зоммерфельда (4.7) и называются уравнениями Липпмана-Швингера. При их анализе используется теория Фредгольма и теорема Като 1.8.

Решения $u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})$ называются стачионарными рассеянными волнами. Они аналогичны решениям $u_j^{(\pm)}(x, k)$ для одномерного случая, где индекс $j = 1, 2$ заменяется вектором $\boldsymbol{\omega} \in S^2$. Абсолютно непрерывный спектр H заполняет $[0, \infty)$ и имеет равномерную бесконечную кратность, параметризованную точками двумерной сферы S^2. Решения $u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})$ - это нормированные собственные функции непрерывного спектра. В общем случае у оператора H есть конечное число отрицательных собственных значений $\lambda_l < 0$ конечной кратности $m_l, l = 1, ..., n$. В терминах операторов $\mathscr{U}_\pm : \mathscr{H} \to \mathscr{H}$, данных формулами

$$\mathscr{U}_\pm(\psi)(\boldsymbol{k}) = (2\pi)^{-\frac{3}{2}} \int\limits_{\mathbb{R}^3} \psi(\boldsymbol{x})u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})d^3\boldsymbol{x},$$

соотношения полноты и ортогональности принимают вид

$$\mathscr{U}_\pm^*\mathscr{U}_\pm = I - P, \quad \mathscr{U}_\pm\mathscr{U}_\pm^* = I,$$

где P - ортогональная проекция на инвариантное подпространство для оператора H, ассоциированное с чисто точечным спектром. Теперь пусть

$$W_\pm = \mathscr{U}_\pm^*\mathscr{U}_0$$

где $\mathscr{U}_0 = \mathscr{F}^{-1}$ - обратное преобразование Фурье. Как и в разделе 3.2.3, можно доказать следующий результат.

Теорема 4.1. Операторы $W_\pm$−волновые операторы для оператора Шрёдингера H. Соответствующий оператор рассеяния $S = W_+^* W_-$ имеет вид

$$S = \mathscr{F}\hat{S}\mathscr{F}^{-1},$$

где $\hat{S}$ - интегральный оператор,

$$(\hat{S}\psi)(k,\boldsymbol{\omega}) = \psi(k,\boldsymbol{\omega}) + \frac{ik}{2\pi}\int\limits_{S^2} f\left(k,\boldsymbol{\omega},\boldsymbol{\omega}'\right)\psi\left(k,\boldsymbol{\omega}'\right)d\boldsymbol{\omega}',$$

$uf\left(k,\boldsymbol{\omega},\boldsymbol{\omega}'\right) = f^{(+)}\left(k,\boldsymbol{\omega},\boldsymbol{\omega}'\right)$
Функция $f\left(k,\omega,\omega'\right)$ называется амплитудой рассеяния.

8.3.5 Properties of the S-Matrix for Scattering in Continuous Media (!?!??)

(пока об этом в отдельной записи, потому что тема очень большая, см. Бязь и др. про рассеяния и распады и сотни статей. Не готов сказать, что из этого на самом деле важно для этой записи.)

8.3.6 Phase Shift Formalism and Partial Cross-Sections

Связь фазовых сдвигов и парциальных сечений по Киселеву

Стационарная волновая функция в задаче рассеяния имеет асимптотический вид

$$\psi_i^{(+)}(r) \simeq e^{ik_i\cdot r} + \frac{e^{\mathrm{i}kr}}{r}f(\theta), \quad k = |\boldsymbol{k}_\mathrm{i}|$$

Разложим амплитуду рассеяния по базису полиномов Лежандра $f(\theta) = \sum\limits_l f_l P_l(\cos\theta)$

Асимптотическое разложение волновой функции по сферическим волнам

$$\psi_i^{(+)}(\boldsymbol{r}) \simeq \sum_l (2l+1)P_l(\cos\theta)\frac{1}{2\mathrm{i}kr}\left\{S_l e^{\mathrm{i}kr} - (-1)^l e^{-\mathrm{i}kr}\right\}$$

С другой стороны, разложение плоской волны свободной частицы и амплитуды рассеяния по полиномам Лежандра дает

$$e^{\mathrm{i}\boldsymbol{k}_\mathrm{i}\cdot\boldsymbol{r}} + \frac{e^{\mathrm{i}kr}}{r}f(\theta) \simeq \sum_l (2l+1)P_l(\cos\theta)\frac{1}{2\mathrm{i}kr}\left\{\left(1+\frac{2\mathrm{i}kf_l}{2l+1}\right)e^{\mathrm{i}kr} - (-1)^l e^{-\mathrm{i}kr}\right\}.$$

Значит,

$$S_l = 1 + \frac{2\mathrm{i}kf_l}{2l+1}$$

и

$$f_l = \frac{(2l+1)}{2\mathrm{i}k}\left(S_l - 1\right)$$

Выражая S_l через фазовые сдвиги

$$S_l = e^{2\mathrm{i}\delta_l},$$

легко находим

$$f_l = \frac{2l+1}{k} e^{\mathrm{i}\delta_l} \sin\delta_l$$

Дифференциальное сечение рассеяния по общей формуле

$$\frac{d\sigma}{d\Omega} = \sum_{l,l'} f_l P_l(\cos\theta) f_{l'}^* P_{l'}(\cos\theta)$$

имеет характерную зависимость от углов, которая и подвергается парциально-волновому анализу при исследовании экспериментальных данных.

В силу ортогональности полиномов Лежандра полное сечение рассеяния

$$\sigma = 4\pi \sum_l \frac{|f_l|^2}{2l+1} = \frac{4\pi}{k^2} \sum_l (2l+1)\sin^2\delta_l$$

Обычно вводят понятие парциального сечения

$$\sigma_l := \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l.$$

Оно принимает максимальное значение при $\delta_l = \pi/2$. Отметим, что для рассеяния вперед $P_l(\cos\theta = 1) = 1$ и

$$\mathrm{Imm} f_l = \frac{2l+1}{k}\sin^2\delta_l$$

так что

$$\sigma_l = \frac{4\pi}{k}\mathrm{Imm} f_l$$

т.е. оптическая теорема справедлива для каждого парциального сечения упругого рассеяния в отдельности.

Свойства фазовых сдвигов по Киселеву

Согласно интегральному уравнению Для амплитуды рассеяния

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\int d^3\boldsymbol{r}' e^{-\mathrm{i}\boldsymbol{k}_E\cdot\boldsymbol{r}'} V(r')\,\psi_{\mathrm{i}}^{(+)}(\boldsymbol{r}')$$

несложно получить выражение и для фазы рассеяния, если воспользоваться разложением по парциальным волнам для волны де Бройля и точного решения стационарного уравнения $\psi_i^{(+)}(\boldsymbol{r})$ с подходящими граничными условиями. В самом деле,

$$e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}'} = \left(\ \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}'\ \right) = 4\pi\sum_{l,m} R_{kl}^{*(0)}(r) Y_{l,m}^*(\boldsymbol{n}')\, Y_{l,m}\left(\boldsymbol{n}^{(k)}\right)$$

где $Y_{l,m}^*(\boldsymbol{n}') = Y_{l,m}^*(\theta',\phi')$, $Y_{l,m}\left(\boldsymbol{n}^{(k)}\right) = Y_{l,m}(\theta,\phi)$, и

$$\psi_i^{(+)}(\boldsymbol{r}') = \sum_{l'}(2l'+1)\,P_{l'}(\cos\theta')\,R_{kl'}(r')$$

так что интегрирование по телесному углу в выражении для амплитуды рассеяния (12.28) элементарно дает

$$\int d\Omega'\cdot Y_{l,m}^*(\theta',\phi')\sqrt{\frac{2l'+1}{4\pi}}P_{l'}(\cos\theta') = \langle l,m|l',0\rangle = \delta_{ll'}\delta_{m0}$$

Поэтому амплитуда выражается в виде ряда

$$f(\theta) = -\frac{2m}{\hbar^2}\sum_l (2l+1)P_l(\cos\theta)\int dr\cdot r^2 R^{*(0)}_{kl}(r)V(r)R_{kl}(r).$$

По определению, парциальные амплитуды имеют вид

$$f_l = -\frac{2m}{\hbar^2}(2l+1)\int dr\cdot r^2 R^{*(0)}_{kl}(r)V(r)R_{kl}(r).$$

Функция $R^{(0)}_{kl}(r)$ - решение одномерного радиального уравнения Шредингера, комплексная фаза которого фиксирована асимптотическим условием

$$R^{(0)}_{kl}(r) \simeq \mathrm{i}^l\cdot\frac{\sin\left(kr-\frac{\pi}{2}l\right)}{kr}$$

так же, как и фаза точного решения стационарного уравнения Шредингера с потенциалом

$$R_{kl}(r) \simeq e^{\mathrm{i}\delta_l}\mathrm{i}^l\cdot\frac{\sin\left(kr-\frac{\pi}{2}l+\delta_l\right)}{kr}$$

Поэтому можно перейти к вещественным волновым функциям $\Phi(r)$ в радиальных уравнения с заданными асимптотикам и на бесконечности, так что

$$R^{(0)}_{kl}(r) = \mathrm{i}^l\cdot\Phi^{(0)}_{kl}(r),\quad R_{kl}(r) = e^{\mathrm{i}\delta_l}\mathrm{i}^l\cdot\Phi_{kl}(r)$$

Тогда

$$f_l = -\frac{2m}{\hbar^2}(2l+1)e^{\mathrm{i}\delta_l}\int dr\cdot r^2\Phi^{(0)}_{kl}(r)V(r)\Phi_{kl}(r)$$

Сравнивая последнее выражение с формулой для парциальной амплитуды в терминах сдвига фазы (13.31), получаем интегральное представление для фазы

$$\sin\delta_l = -\frac{2mk}{\hbar^2}\int dr\cdot r^2\Phi^{(0)}_{kl}(r)V(r)\Phi_{kl}(r)$$

В борновском приближении, очевидно,

$$\sin\delta_l \approx -\frac{2mk}{\hbar^2}\int dr\cdot\left\{r\Phi^{(0)}_{kl}(r)\right\}^2 V(r)$$

Интегральное представление позволяет установить некоторые свойства сдвигов фаз, причем, поскольку основные свойства радиальных волновых функций для свободных волн и вблизи нуля и периоду осцилляций практически совпадают, Выводы о парциальных амплитудах, сделанные на основе борновского приближения и точного интегрального представления, мало отличаются друг от друга, за исключением важного случая резонансов.

Пусть потенциал имеет характерную величину $|V| \simeq V_0$, и он существенно отличен от нуля только в области $r < a$. Как мы выяснили, вблизи нуля поведение радиальной волновой функции

$$R_{kl} \sim (rk)^l\frac{(2l)!!}{(2l+1)!} \sim (rk)^l\frac{2^l l^l e^{-l}\sqrt{2\pi l}}{(2l+1)^{2l+1}e^{-2l-1}\sqrt{2\pi(2l+1)}} \sim \left(\frac{erk}{2l}\right)^l \sim \left(\frac{rk}{l}\right)^l$$

где мы воспользовались формулой Стирлинга для оценки факториалов и опустили несущественные числовые множители.

При этом удобно считать для общности рассмотрения, что эти выражения остаются справедливыми и при $l \to 0$, если формально положить $l^l \to \text{const}$.

В Оправданности чего можно убедиться, непосредственно подставив $R_{k0} \sim \text{const}$.

Значит, интеграл, определяющий фазу, можно оценить как

$$\int dr \cdot \left\{ r\Phi_{kl}^{(0)}(r) \right\}^2 V(r) \sim \frac{a^2 V_0}{k} \left(\frac{ak}{l} \right)^{2l+1}$$

откуда

$$\sin \delta_l \sim \frac{2mV_0}{\hbar^2} a^2 \left(\frac{ak}{l} \right)^{2l+1} \qquad \text{и} \qquad \sin \delta_0 \sim \frac{2mV_0}{\hbar^2} a^3 k$$

Из этих оценок заключаем, что рассеяние частиц с $l \gg ka$ подавлено. Этот ϕ акт согласуется с классически м рассмотрением, поскольку орбитальный момент падающей на мишень частицы можно оценить как произведение волнового вектора (импульса) на прицельное расстояние b, так что при

$$l \sim kb \gg ka \to b \gg a$$

т.е. прицельное расстояние много больше радиуса действия потенциала, и рассеяния не происходит.

С другой стороны, малый вклад в сечение парциальных волн с $l \gg ka$ можно понять, исходя из относительного вклада центробежного потенциала в энергию частицы при больших $l \gg 1$

$$\frac{\Delta V_l(r)}{E} = \frac{\hbar^2 l^2}{2mEr^2} \approx \left(\frac{l}{kr} \right)^2$$

Значит, вклад орбитального момента в энергию радиального движения создает при $r = a$ потенциальный барьер относительной высоты

$$\frac{l^2}{(ka)^2}$$

При $l \ll ka$ происходит надбарьерное рассеяние, и частица достигает потенциала, отличного от нуля при $r < a$. При $l \gg ka$ проницаем ость Высокого и шпрокого барьера сильно подавлена, вероятность проникновения на расстояния $r < a$ крайне мала, так что частица практически рассеивается также, как и в случае свободного движения: вклад области, где существенно наличие потенциала, пренебрежимо мал, т.е. фазы рассеяния близки к нулю.

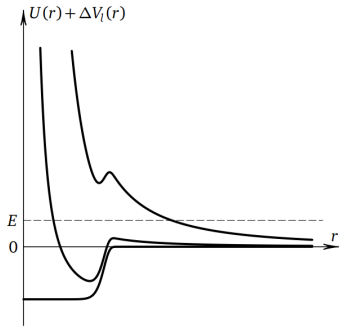


Figure 8.1: Потенциал радиального движения для $l = 0$ (нижняя кривая), $l = 0,7ka$ (средняя кривая) и $l = 2ka$ (верхняя кривая)

Отличие квантового описания рассеяния от классического

(четко опишу, какое оно?)

8.3.7 Scattering of Identical Particles

(см пока лекцию Киселева, там пара страниц нетривиальных мыслей)

8.3.8 Scattering on Coulomb Potential

(типично это решается отдельно, ибо особенностей много. скоро выпишу из Тонга!)

Main theory

Experiments on Coulomb scattering

(графики и эксперименты опишу)

Другие свойства кулоновского рассеяния

Two-dimensional coulomb scattering of a quantum particle: wave functions and green's functions by v. V. Pupyshev (2016)

(есть статья на 18 страниц, где получено много сложных формул. Не уверен, что они нужны, но если нужны будут - допишу сюда. Впечатление от статьи: там возня со спецфункциями, нужно пару дней про это думать, чтобы понять, как вообще их применять. Ну и вряд ли приложения этой теории есть. Пока сам это не могу сделать - пусть заготовка побудет)

Annotation:

We solve the problem of the propagation of a charged quantum particle in a two-dimensional plane embedded in the three-dimensional coordinate space. We consider scattering of this particle by a stable Coulomb center situated in the same plane. We study the wave function of this particle, its Green's function, and all radial components of these functions. We derive uniform majorant bounds on absolute values of these functions and find the wave function representation in terms of regular radial Coulomb functions and the scattering amplitude representation via partial phases. We obtain integral representations of the Greens's function and all its radial components.

8.3.9 Illustrative Examples of Typical Scattering Models

(для больших примеров - см. задачи, а для особых ситуаций - см. дальнейшие части и разделы)

8.3.10 Comparison of Quantum and Classical Scattering Theories

(проведу анализ. уже это многим делалось. конкретные примеры и графики добавлю!)

8.4 Analytical Properties of Physical Quantities

(это перенесу скорее всего в другие записи, потому что квантмех тут вообще не везде.)

Все физические величины при реальных значениях параметров не должны обращаться в бесконечность. Иными словами, на вещественной оси в реально достижимых областях физические функции конечны. Единственные допустимые особые точки - это точки ветвления. В каждом случае для их появления должны быть физические причинь.

В комплексной плоскости параметров физические функции могут иметь различные особые точки. Однако всегда можно выделить области, в которых функции аналитичны.

Из свойств аналитичности можно делать важные заключения о связях между различными физическими величинами. Рассмотрим несколько примеров.

8.4.1 Dependence of the Nuclear Moment of Inertia on Deformation

Для квантовомеханической сферической системы момент инерции равен нулю, так как ее вращение не имеет физического смысла. Рассиотрим момент инерции J при малых деформацнлх (??). С какого члена начинается разложение J по степеням δ? Легко убедиться в том, что выражение $J = A\delta$ неправильно. Предположим, что $J = A\delta$ для положительных δ («огурец»). Так как J всегда положительная величина, то для отрицательных δ («блин») по принципу аналитического продолжения $J = A|\delta| = A\sqrt{\delta^2}$. Следовательно, момент инерции как функция δ^2 имел бы в нуле точку ветвления. Между тем, можно убедиться, что нет никаких причин для появления особой точки. Действительно, перейдем от слабо деформированного ядра к сферическому с помощью соответствующего преобразования координат. В гамильтониане появится малая добавка H', пропорииональная величине деформации δ. Для конечной системы применение теории возмущений дает сходящийся ряд. Следовательно, момент инерции не имеет особой точки при $\delta = 0$. Поэтому разложение J по степеням δ начинается с квадратичного члена

$$J = B\delta^2 + ...$$

(??? потом про это еще подумаю.)

8.4.2 Dependence of Sound Frequency on the Wave Vector

Как известно, при малых волновых числах k (т. е. больших длинах волн $\lambda\!\!\!^{-} = 1/k$) в некоторых системах могут распространяться звуковые возбуждения с частотой $\omega = ck$. Здесь c - скорость звука. Так как ω - скаляр, а $\boldsymbol{k}$ - вектор, то это соотношение означает $\omega = c\sqrt{\boldsymbol{k}^2}$. Итак, при $k = 0$ частота ω как функция k^2 имеет точку ветвления. Объясним, почему здесь возникает особая точка.

Уравнения, описывающие состояние системы, инвариантны при замене $t \longrightarrow -t$, если нет диссипации. Поэтому уравнение для определения частоты всегда содержит ω^2, а не ω. Например, в классической механике уравнение Ньютона для каждой колеблющейся частицы при малых колебаниях имеет вид

$$m\ddot{u}_n = -\sum_m F_{mn}u_m.$$

Здесь m - масса n-й частицы, u_n - ее смещение, а F_{mn} сила, действующая на n-ю частицу со стороны m-й. Полагая $u_n = u_{0n}e^{i\omega t}$, получим дисперсионное уравнение для квадрата частоты звука ω^2 в виде

$$m\omega^2 u_{0n} = \sum_m F_{mn}u_{0m}.$$

Следовательно, квадрат частоты ω^2, а не сама частота ω, должен быть аналитической функцией параметров задачи. Поэтому

$$\omega^2 = a + c^2k^2 + bk^4 + ...$$

Для звуковых волн $a = 0$, следовательно, для малых k частота $\omega = c|\boldsymbol{k}|$.

8.4.3 Analytical Properties of the Wave Function

(??? maybe move it to the part of basics)

Движение частицы в поле с потенциалом $V(r)$ определяется волновой функцией Ψ, которая подчиняется уравнению Шредингера:

$$-\frac{1}{2}\Delta\Psi + V\Psi = E\Psi$$

Для сферически-симметрического потенциала $V(r)$ радиальная и угловые переменные разделяются, т. е.

$$\Psi = R_{nl}(r)Y_{lm}(\theta,\varphi),$$

причем $R_{nl}(r)$ удовлетворяет уравнению

$$R'' + \frac{2}{r}R' + 2\left[E - V - \frac{l(l+1)}{2r^2}\right]R = 0.$$

Обозначим $V_l = V + \frac{l(l+1)}{2r^2}$ и заменим $R = \frac{u}{r}$. Тогда для u получается следующее уравнение:

$$u'' + 2\left(E - V_l\right)u = 0.$$

Так как волновая функция R во всех точках пространства конечна, то $u(0) = 0$.

Известно, что особые точки решения линейного дифференциального уравнения всегда совпадают с особыми точками коэффициентов уравнения (кроме бесконечно удаленной особой точки). Однако особые точки коэффициентов могут и не быть особыми точками решения. Например, в уравнении (1.14) точка $r = 0$-особая точка коэффициента уравнения, так как $V_l \to \infty$. Если $l \neq 0$, то при малых r можно пренебречь $V(r)$ по сравнению $l(l+1)/r^2$. Следовательно, уравнение (1.14) приобретает вид $r^2u'' - l(l+1)u = 0$, откуда $u_1 \sim r^{l+1}$ или $u_2 \sim r^{-l}$. Итак, существует решение $u_1 \sim r^{l+1}$, которое не обращается в бесконечность при $r \longrightarrow 0$. $\underset{r\to 0, l\neq 0}{}$

Итак, особые точки решения уравнения Шредингера (1.14) могут быть только там, где потенциал имеет особенность.

Например, осцилляторный потенциал $V = \frac{1}{2} \propto x^2$ имеет особую точку на бесконечности. Поэтому и решение имеет особую точку только на бесконечности.

Кулоновский потенциал, рассматриваемый как функция r^2, имеет особенность при $r^2 = 0$. По этой причине радиальные функции имеют особенность при $r^2 = 0$, а именно, $R_{nl}\left(r^2\right)$ имеет в нуле точку ветвления (например, функция основного состояния $R \sim e^{-Vr^2}\Big)$. Ниже (стр. 53) мы увидим, что эта особенность кулоновских функций приводит к важным следствиям. (!??!?!?)

8.4.4 Scattering Amplitude at Low Energies

Ψ-функция при больших r в задаче рассеяния имеет асимптотический вид

$$\Psi \underset{r\to\infty}{\to} e^{ikz} + \frac{f}{r}e^{ikr},$$

где f - амплитуда рассеяния.

Предположим для простоты, что рассеяние сферически-симметрично, т. е. f не зависит от углов. Рассмотрим сферически-симметричную часть Ψ:

$$\int \Psi\frac{d\Omega}{4\pi} \equiv \frac{u}{r} = \frac{1}{2}\int_0^\pi e^{ikr\cos\vartheta}\sin\vartheta d\vartheta + \frac{f}{r}e^{ikr} = \left(\frac{\sin kr}{k} + fe^{ikr}\right)\frac{1}{r}.$$

Функцию u можно представить в виде

$$u = -\frac{1}{2ik}e^{-ikr} + \frac{1+2ikf}{2ik}e^{ikr}.$$

Если рассеивающий центр не поглощает и не испускает частиц, то радиальный ток частиц равен нулю. Перекрестные члены сокращаются, и оказывается, что ток равен разности токов, составленных из двух слагаемых и. Условие равенства этик двух токов дает

$$|1+2ikf|^2 = 1,$$

или, иначе,

$$f - f^* = 2ikff^*, \quad \operatorname{Im} f = k|f|^2$$

откуда получаем

$$\operatorname{Im}\frac{1}{f} = -k, \quad f^{-1} = \varkappa - ik,$$

где $\varkappa$ - вещественное число.

Величину $\varkappa$ можно выразить через энергию связанного состояния частицы в рассеивающей яме (если такое состояние существует). Действительно, функция ι может быть аналитически продолжена из области положительных энергий в область отрицательных, что соответствует мнимым значениям $\boldsymbol{k}$. Пусть энергия связанного состояния равна $(-E_0)$. Обозначим $x_0 = \sqrt{2E_0}$. Тогда при $k = \pm ix_0\Psi$-функция для положительных энергий должна переходить в Ψ-функцию связанного состояния. Поэтому в выражении для u при $k = \pm i\varkappa_0$ не должно оставаться слагаемого с растущей экспонентой.

Подставляя (1.17) в выражение (1.15), получим

$$u = -\frac{1}{2ik}\left(e^{-ikr} + \frac{x+ik}{x-ik}e^{ikr}\right).$$

При $\Leftrightarrow= ix_0$ получаем

$$u = \frac{1}{2x_0}\left(e^{x_0 r} + \frac{x-x_0}{x+x_0}e^{-x_0 r}\right).$$

Для того чтобы можно было пренебречь растущей экспонентой, необходимо $x = -\varkappa_0$. При $k = -ix_0$ получается это же условие. Таким образом, амплитуда рассеяния имеет полюс

$$f = -\frac{1}{x_0 + ik},$$

положение которого определяется энергией связанного состояния.

8.4.5 Analytical Properties of a Dielectric Constant

Аналитичность некоторых физических величин, как мы увидим, есть следствие причинности.

Рассмотрим, например, аналитические свойства диэлектрической постоянной. Индукция $D(t)$, возникающая в системе при наложении электрического поля, определяется амплитудой поля E во все предыдущие моменты времени $t - \tau(\tau > 0)$. Итак,

$$D(t) = \int_0^\infty K(\tau)E(t-\tau)d\tau$$

$K(\tau)$ - вещественная функция, так как она связывает физические величины. Это соотношение вытекает лишь из того, что следствие наступает позже причины. Разложим E и D в ряды Фурье:

$$E = \int E_\omega e^{-i\omega t} d\omega, \quad D = \int D_\omega e^{-i\omega t} d\omega.$$

Тогда из (1.19) находим

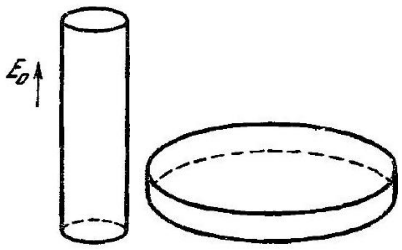
$$D_\omega = E_\omega \int_0^\infty K(\tau) e^{i\omega\tau} d\tau,$$

откуда диэлектрическая постоянная

$$\varepsilon_\omega = \frac{D_\omega}{E_\omega} = \int_0^\infty K(\tau) e^{i\omega\tau} d\tau.$$

Величина ε_u аналитична в верхпей полуплоскости комплексной переменіой ω. Действительно, если обозначить $\omega = \omega_0 + i\omega_1$, где $\omega_1 > 0$, то подынтегральное выражение в (1.20) содержит затухающую эксионенту $e^{-\omega_1\tau}$, и ноэтому интеграл (1.20) сходится, а следовательно, представляет аналитическую функцию.

Нетрудно видеть, что аналитические свойства $\boldsymbol{\varepsilon}$ и $1/\varepsilon$ совнадают. Рассмотрим длинный и короткий цнлиндры вещества, на которые наложено внешнее поле E_0 (рнс. 8).

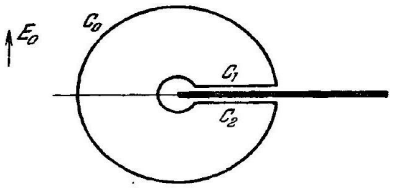


В случае длинного цилиндра поле внутри E равняется внешнему полю E_0, а индукция $D = \varepsilon E_0$. В случае короткого цилиндра индукция D равняется внешнему полю E_0, а поле внутри $E = E_0/\varepsilon$. В первом случае $D = \int_0^\infty K_1(\tau) E_0(t-\tau) d\tau$ и $\varepsilon = \int_0^\infty K_1(\tau) e^{i\omega t} d\tau$. Во втором случае поле E определяется значеннями $E_0 = D$ в предыдущие моменты времени, $E = \int_0^\infty K_2(\tau) D(t-\tau) d\tau$, откуда $1/\varepsilon = \int_0^\infty K_2 e^{i\omega\tau} d\tau$. Таким образом, аналитические свойства е и $1/\varepsilon$ совпадагот. Следовательно, диэлектрическая постоянная не имеет ни полдосов, ни нулей в верхней полуглоскости.

Так как $\varepsilon(i\omega_1) \underset{\omega_1>0}{\Rightarrow} \int_0^\infty K(\tau) e^{-\omega_1\tau} d\tau$, то ввиду веществеппостн поднптегрального выражения и $\varepsilon(i\omega_1)\,|\omega_1 > 0$ вещественна, т. е. $\operatorname{Im}\varepsilon(i\omega_1) = 0$

$\omega_1 > 0$

Используя аналигичпость, можно выразить вещественную часть диэлектрической постояпной через ее мнимую часть. Рассмотрим комплексную плоскость ω^2. В этом случае область аналитичности ε представляет собой первый лист римановони илоскости - все особые точки лежат на втором листе. Первый лист переходит во второй через разрез, идущий вдоль положительных ω^2 от точки $\omega^2 = 0$ (рис. 9).



Согласно теореме Коши

$$f(z) = \frac{1}{2\pi i} \int\limits_C \frac{f(z')\,dz'}{z - z'}$$

где C-замкнутый контур, не содержащий внутри себя особых точек $f(z)$. Применим эту теорему к $\varepsilon(\omega)^2)$, взяв в качестве C контур, изображенный на рис. 9. При больших ω^2, как мы увидим, $\varepsilon\left(\omega^2\right)$ имеет вид $\varepsilon \to 1 - \frac{c_1}{\omega^2}$. Поэтому для того, чтобы интеграл по контуру C_0 обращался в нуль, нужно в качестве f взять функцию $f = \varepsilon - 1$. Итак,

$$\varepsilon\left(\omega^2\right) - 1 = \frac{1}{2\pi i} \int \frac{\varepsilon\left(\omega_1^2\right) - 1}{\omega_1^2 - \omega^2} d\omega_1^2.$$

Кз рис, 9 видно, что этот интеграл сводится к обходу разреза. Обозначим через $\varepsilon_1\left(\omega^2\right)$ значение ε на верхнем берегу разреза, а через $\varepsilon_2\left(\omega^2\right)$ значение ε на нижнем берегу. Покажем, что $\varepsilon_2\left(\omega^2\right) = \left[\varepsilon_i\left(\omega^2\right)\right]^*$. Мы видели, что & вещественно на мнимой верхней полуосія плоскости. п. Следовательно, в плоскости ω^2 величина ε вещественна на полуосн $\omega^2 < 0$. Продолжая аналитически это соотношение на верхний и нижний берега разреза, получаем

$$\varepsilon_1\left(\omega^2\right) = \left[\varepsilon_2\left(\omega^2\right)\right]^* |\omega^2 > 0.$$

Учитывая (1.22), из (1.21) находим

$$\varepsilon\left(\omega^2\right) - 1 = \frac{1}{2\pi i} \int\limits_{C_1} \frac{\varepsilon_1\left(\omega_1^2\right) - \varepsilon_3\left(\omega_1^2\right)}{\omega_1^2 - \omega^2} d\omega_1^2 = \frac{1}{2\pi} \int\limits_{C_1} \frac{2\,\mathrm{Im}\,\varepsilon\left(\omega_1^2\right) d\omega_1^2}{\omega_1^2 - \omega^2}.$$

Итак,

$$\varepsilon\left(\omega^2\right) = 1 + \frac{1}{\pi} \int\limits_0^\infty \frac{\mathrm{Im}\,\varepsilon\left(\omega_1^2\right) d\omega_1^2}{\omega_1^2 - \omega^2},$$

т. е., зная мнимую часть диэлектрнческой постоянной ε, можно восстановить всю величину ε.

Мнимая часть диэлектрической постояиной, определяюиая поглощение электромагнитных волн системо, отлична от нуля только, когда частота волн совпадаст с собствннымн частотамн системы ω_n. Иными словами,

$$\mathrm{Im}\,\varepsilon\left(\omega^2\right) = \sum_n \pi f_n \delta\left(\omega^2 - \omega_n^2\right).$$

Подставляя (1.24) в (1.23), получаем

$$\varepsilon\left(\omega^2\right) = 1 + \sum_n \frac{f_n}{\omega_n^2 - \omega^2}$$

При $\omega^2 \gg \omega_n^2$ величина ε должна перейти в диэлектрическую постоянную идеального газа электронов, т. е. $\varepsilon \underset{\omega^2 \to \infty}{\longrightarrow} 1 - \frac{4\pi n e^2}{m\omega^2}$, где n - число электронов в единице объема, а m - масса электрона. Таким образом, из (1.23) и (1.25) получаем

$$\frac{1}{\pi}\int \operatorname{lm}\varepsilon\left(\omega_1^2\right)d\omega_1^2 = \frac{4\pi n e^2}{m} = \sum_n f_n.$$

Это соотношение называется правилом сумм.

(по идее это должен я уже хорошо знать, но пока еще не отработал, потом потренируюсь. типичная такая тема.)

8.4.6 Analytical Properties of a Scattering Amplitude

Аналогичным способом доказываются аналитические свойства амплитуды рассеяния. Рассмотрим, например, рассеяние света заряженной системой. Пусть амплитуда рассеянной волны характеризуется величиной B, а падающей - A. Эти величины связаны друг с другом соотношением

$$B(t) = SA(t),$$

где S - некоторый интегральный оператор. Сделаем предположение, что до момента времени $t = 0$ амплитуда падающей волны на некоторой контрольной плоскости, расположенной до рассеивающей системи, равна нуло. Относительно B можно утверждать, что $B(t) = 0$ для $t < t_1$, где $t_1 > 0$.

Перейдем к фурье-компоненте $A_\omega = \int\limits_0^\infty A(t)e^{i\omega t}dt$. Так как $A(t) = 0$ при $t < 0$, то A_ω не имеет особенностей в верхней полуплоскости. Аналогично имеем $B_\omega = \int\limits_{t_x>0}^\infty B(t)e^{i\omega t}dt$, т. е. B_ω также не имеет особенностей в верхней полуплоскости. Из (1.26) следует, что $B_\omega = SA_\omega$.

Отсюда видно, что величина S может иметь особенности лишь в нулях A. Но S не может зависеть от частного вида A, следовательно, S вообще не может иметь особенностей в верхней полуплоскости. Оператор S линейно связан с амплитудой рассеяния f света. Поэтому дисперсионное соотношение для f аналогично дисперсионному соотношению для диэлектрической постоянной ε (напомним, что $\varepsilon\left(\omega^2\right) = 1 + \frac{1}{\pi}\int\limits_0^\infty \frac{\operatorname{Im}\varepsilon\left(\omega_1^2\right)d\omega_1^2}{\omega_1^2-\omega^2}$):

$$f\left(\omega^2\right) = \frac{1}{\pi}\int \frac{\operatorname{Im} f\left(\omega_1^2\right)d\omega_1^2}{\omega_1^2-\omega^2}$$

В случае рассеяния света заряженной системой такое выражение для амплитуды неверно, так как амплитуда при больших частотах стремится не к нулю, а к сумме амплитуд рассеяния на свободных частицах. Поэтому дисперсионное соотношение нужно применять не к величине f, а к величине $f\left(\omega^2\right) - f(\infty)$ аналогично тому, как это делалось в случае диэлектрической постоянной. (!?!?!!??!?!)

8.5 Scattering theory: Other features and methods

8.5.1 Eikonal Approximation (??)

(нужно додумывать, не типичная теория)

Конструкция эйконального приближения по Зинн-Жюстену

Решение, удовлетворяющее граничным условиям представления (9.11) и соответствующее свободному гамильтониану

$$H_0 = \mathrm{p}^2/2m, \text{ где } \mathrm{p} \in \mathbb{R}^d$$
$$\mathrm{q}(t) = \mathrm{q}' + (\mathrm{q}'' - \mathrm{q}')\,\tfrac{t-t'}{t''-t'}$$

После сдвига переменных интегрирования $\mathrm{q}(t)$ на классическое решение (9.36) вычисление сводится к нормировочному интегралу, который может быть определен сравнением с точным результатом ($\hbar = 1$)

$$\langle \mathrm{q}''|U\left(t'',t'\right)|q'\rangle = \left(\frac{m}{2i\pi\left(t''-t'\right)}\right)^{d/2} \exp\left[i\frac{m}{2}\frac{\left(q''-q'\right)^2}{\left(t''-t'\right)}\right].$$

Эйкональное приближение соответствует кинематическому режиму

$$p' = p - k/2, \quad p'' = p + k/2, \quad p^2 \to \infty, \quad p^2 \gg k^2$$

В этом случае в действии кинетический член преобладает над потенциальным.

Поэтому будем вычислять континуальный интеграл тах же, как и в свободном случае, разлагая траектории вблизи классической траекторий свободного движения (9.36).

Вычисление оператора эволюции в ведущем порядке достаточно просто.

Полагая $q'' - q' = s(q'' + q')/2 = x$, получим:

(упущена формула) 9.38

классическое действие теперь имеет вид:

$$A(s,x) = \frac{im}{2}\frac{s^2}{t''-t'} - i\int\limits_{t'}^{t''} dtV\left(x - \frac{s}{2} + \frac{t-t'}{t''-t'}s\right)$$

а нормировка в равенстве (9.38) определяется сравнением с результатом (9.37), отвечающим свободному движению.

В пределе большого временного интервала, если пренебречь вкладом потенциального слагаемого, основной вклад в интеграл по s дает седловая точка

$$\mathrm{s} = \left(t''-t'\right)\mathrm{p}/m$$

После подстановки s и замены переменных $t - \left(t'+t''\right)/2 \mapsto t$, такой, что $|t| \leqslant \left(t''-t'\right)/2$, аргумент потенциала принимает вид $\mathrm{x} + \mathrm{tp/m}$.

Будем считать, что потенциал достаточно быстро убывает, чтобы существовал предел интеграла в (9.39) при больших временах, т.е. при $t''-t' \to \infty$. Вклад потенциала в действие в этом случае имеет вид

$$-i\int\limits_{-\infty}^{+\infty} dtV(\mathrm{x} + t\mathrm{p/m})$$

Как только мы перешли к пределу, можно сдвинуть переменную интегрирования t, не меняя область интегрирования.

Это сводится к сдвигу вектора x в аргументе потенциала V на вектор, пропорциональный .

Выберем этот вектор так, чтобы V зависел только от

$$b = x - p\left(x \cdot p/p^2\right)$$

- компоненты x, ортогональной p.

Тогда интеграл по компоненте x вдоль p может быть вычислен, и из него следует условне $\mathrm{p} \cdot \mathrm{k} = 0$. В области применимости эйконального приближения это равенство выражает закон сохранения энергии:

$$0 = \mathrm{p}''^2 - \mathrm{p}'^2 = (\mathrm{p} + \mathrm{k}/2)^2 - (\mathrm{p} - \mathrm{k}/2)^2 \sim 2\mathrm{p} \cdot \mathrm{k}$$

Получим:

$$\langle \mathrm{p} + \mathrm{k}/2 \left| U\left(t'', t'\right) \right| \mathrm{p} - \mathrm{k}/2) \simeq \delta(\mathrm{p} \cdot \mathrm{k}) \mathcal{N}(\mathrm{p}) \int d^{d-1} b e^{-ik \cdot b} \exp\left[-i \int\limits_{-\infty}^{+\infty} dt V\left(\frac{\mathrm{p}t}{m} + \mathrm{b}\right)\right],$$

$$\mathcal{N}(\mathrm{p}) \sim \exp\left[i\left(t'' - t'\right) \frac{\mathrm{p}^2}{2m}\right]$$

Равенство (9.42) дает после преобразования Фурье матричные элементы оператора рассеяния T в импульсном базисе (определенные равенством (9.9)) :

$$\langle \mathrm{p} + \mathrm{k}/2 | T | \mathrm{p} - \mathrm{k}/2 \rangle \simeq \frac{i|\mathrm{p}|}{m} \int \frac{d^{d-1} b}{(2\pi)^d} e^{-i\mathrm{k} \cdot \mathrm{b}} \left\{ \exp\left[-i \int\limits_{-\infty}^{+\infty} dt V\left(\frac{\mathrm{p}t}{m} + \mathrm{b}\right)\right] - 1 \right\}$$

Через Фурье-представление

$$V(\mathbf{q}) = \int d^d s e^{iq \cdot s} \tilde{V}(\mathrm{~s})$$

Интеграл от потенциала может быть записан в виде:

$$\int\limits_{-\infty}^{+\infty} dt V\left(\frac{\mathrm{p}t}{m} + \mathrm{b}\right) = \int d^d s \widetilde{V}(\mathrm{~s}) \int\limits_{-\infty}^{+\infty} dt e^{\mathrm{i}(\mathrm{p}t/m + \mathrm{b}) \cdot \mathrm{s}}$$

Интеграл по времени теперь можно взять и свести интеграл по интегралу по компонентам s, ортогональным p:

$$\int\limits_{-\infty}^{+\infty} dt V\left(\frac{\mathbf{p}t}{m} + \mathbf{b}\right) = 2\pi \frac{m}{|\mathbf{p}|} \int d^d s \delta(\mathbf{s} \cdot \widehat{\mathbf{p}}) e^{i\mathbf{b} \cdot \mathbf{s}} \tilde{V}(\mathrm{~s})$$

В это выражение входит Фурье-образ $\widetilde{V}$, но в $(d-1)$ -мерном подпро странстве, ортогональном p Наконец, отметим, что в ведущем порядке по V эйкональное при ближение сводится к

$$\langle \mathbf{p} + \mathbf{k}/2 | T | \mathbf{p} - \mathbf{k}/2 \rangle = \tilde{V}(\mathbf{k})$$

т.е. к точному борновскому приближению (см. Раздел 9.2).

Применение эйконального приближения к кулоновскому потенциалу

Применим теперь эйкональное приближение к нахождению амплитуды рассеяния в случае потенциала вида $1/q$ - кулоновского типа.

В этом случае интеграл от потенциала не имеет предела для бесконечного временного интервала, потому что потенциал слишком медленно убывает на больших расстояниях.

Поэтому необходимо сначала интегрировать по конечному временному интервалу.

Параметризуем потенциал следующим образом:

$$V(\mathbf{q}) = \frac{\alpha}{|\mathbf{q}|}$$

Тогда

$$\int\limits_{(t'-t'')/2}^{(t''-t')/2} \mathrm{d}t V\left(\frac{\mathbf{p}t}{m} + \mathbf{x}\right) \simeq \frac{2\alpha m}{p} \ln\left(\left(t''-t'\right) p/mb\right)$$

Эта бесконечная фаза имеет следующее происхождение: так как кулоновский потенциал слишком медленно убывает на больших рас стояниях, классическая траектория слишком медленно приближает к траектории свободного движения, которая при нашем определенi, S -матрицы принята в качестве эталонной.

В кулоновском потенциале амплитуды не определены - определены только сечения.

Факторизуя бесконечную фазу, можно завершить вычисление зм: плитуды рассеяния.

Интегрируя по вектору b, получим:

$$T(\mathbf{p}+\mathbf{k}/2, \mathbf{p}-\mathbf{k}/2) \simeq \frac{i\pi^{(d-1)/2}}{(2\pi)^d} \frac{p}{m} \exp\left[-i\frac{2\alpha m}{p} \ln\left(\left(t''-t'\right) p/m^b\right)\right] \frac{\Gamma\left[\frac{1}{2}(d-1)-\theta\right]}{\Gamma(\theta)} \left(\frac{k^2}{4}\right)^{[\theta+(1-d)/2)}$$

rде $\theta = -iam/p$. В физической размерности з выраженне (9.47) совпадает с точным результатом.

При $\alpha < 0$ (случай притяжения) оно дает энергин E_n связанных состояний в кулоновском потенциале, которые проявляются в виде полюсов амплитуды рассеяния:

$$\theta = \frac{1}{2}(d-1) + n \to E_n = \frac{\mathrm{p}^2}{2m} = -\frac{2\alpha^2 m}{(d-1+2n)^2}$$

Узнается хорошо известный кулоновский спектр.

Наконец, эйкональное приближение обладает релятивистским обоб- щением, которое дает очень интересные приближения для спектра энергий в квантовой электродинамике.

В последнем случае оно состоит в приближенном суммировании лестничных и перекрестных лестничных диаграмм Фейнмана.

Теория возмущений и операторы

Чтобы проиллюстрировать соответствие между формулировкой квантовой механики с помощью континуального интеграла и операторной формулировкой, напомним основы теории возмущений в операторном формализме для случая не зависящих от времени гамильтонианов.

Разложение S -матрицы может быть получено, например, из разложения оператора (см. (9.6))

$$\Omega(t) = e^{iH_0 t} e^{-iHt}$$

где H_0 - невозмущенный гамильтониан, и

$$V = H - H_0$$

возмущение.

Вводя оператор возмущения в представлении взаимодействия

$$V_1(t) = e^{iH_0 t} V e^{-iH_0 t}$$

можно убедиться, что оператор $\Omega(t)$ удовлетворяет уравнению

$$\dot{\Omega}(t) = -iV_1(t)\Omega(t)$$

граничным условием

$$\Omega(0) = 1$$

(допишу потом)

Применения эйконального приближения

(потом разберу, это важно)

8.5.2 Resonances

Резонансы по Киселеву

(добавлю напоминание, что происходит вообще?)

Парциальное сечение достигает своего макси мума $\sigma_l = 4\pi(2l+1)/k^2$ при Энергии, когда $\delta_l = \pi/2$. В этом случае говорят о наличии резонанса в l -канале.

Запишем Парциальную амплитуду

$$\frac{k}{2l+1} f_l = \frac{\sin\delta_l}{e^{-\mathrm{i}\delta_l}} = \frac{\sin\delta_l}{\cos\delta_l - \mathrm{i}\sin\delta_l} = \frac{1}{\operatorname{ctg}\delta_l - \mathrm{i}}$$

Котангенс парциального сдвига δ_l обращается в нуль, если энергия близка к резонансной $E \approx E_*$, Т.е.

$$\operatorname{ctg}\delta_l \approx 2\frac{E_* - E}{\Gamma}$$

где мы ввели величину размерности энергии Γ и положили, что в ведущем приближении Зануление происходит линейно по энергии.

Значит,

$$\delta_l \approx \arctan\frac{\Gamma}{2\,(E_* - E)}$$

при вариации энергии вблизи резонанса в малой области размером в несколько Γ пробегает Значения от нуля до π. Для парциальной фазы можно записать

$$\frac{k}{2l+1} f_l = \frac{e^{2\mathrm{i}\delta_l} - 1}{2\mathrm{i}} = \frac{\mathrm{i}}{2} - \frac{\mathrm{i}}{2} e^{2\mathrm{i}\delta_l}$$

Это показывает, что в Комплексной плоскости парциальная амплитуда с ростом энергии пробегает против часовой стрелки по окружности, центр которой смещен из нуля на чисто мнимую ось, как это показано на рис.

9.5.

Подобный график называют "Арганд-плот".

Окружность на таком графике практически замкнутая, если вдали от резонанса сдвиг фазы относительно мал.

Парциальное сечение рассеяния вблизи резонанса как функция энергии приобретает Зависи мость брейт-вигнеровского типа

$$\sigma_l = \frac{\pi(2l+1)}{k^2(E)} \frac{\Gamma^2}{(E_* - E)^2 + \Gamma^2/4}$$

т.е. имеет вид пика с ширин ой на полувысоте Г.

Однако пикообразная форма зависи мости сечения от энергии сама по себе может возникать по различным динамическим причинам, поэтому для идентификации резонансов при парциально-волновом анализе экспериМентальных данных по рассеянию поточечно строят Арганд-плот, что в случае характерной

Зависи мости и служит достоверным доказательством наличия резонанса в том или ином канале.

Выше мы молчаливо полагали, что ширина Г положительна.

Это отвечает том у, что аамплитуда рассеяния

$$\frac{k}{2l+1} f_l \approx \frac{\frac{\Gamma}{2}}{E_* - E - \mathrm{i}\frac{\Gamma}{2}}$$

и меет полюс в комплексной плоскости энергии при $E = E_* - \mathrm{i}\Gamma/2$, т.е. полюс смещен в нижнюю полуплоскость.

Этот вопрос тесно связан с исследовани ем аналитических свойств как амплитуд рассеяния, так и функции Грина стационарн ого уравнения Шредингера, что Выходит за рамки нашего изложения.

Вкратце же отметим, что, в частности, на примере функции Грина свободной частицы мы видели, что по энергии она и меет разрез в комплексн ой плоскости вдоль вещественной оси от нуля до бесконечности, т.е.

при значениях энергии в непрерывн Ом спектре.

При наличии связанных состояний функция Грина, как следует из разложения по базису стационарных состояний, приобретает полюса на вещественной оси в точках дискретного спектра.

Резонансы имеют место в непрерывн Ом спектре, так что отмеченный полюс расположен "за" разрезом, т.е.

на нефизическом листе двулистной функции Г рина, зависяшей от $k = \sqrt{2mE/\hbar^2}$

Арганд-плот и его применения

Наконец, отметим, что резонанс при наличии неупругих каналов рассеяния на "Арганд-плоте" проявляется в Виде витка неправильной спирали.

(тут укажу, где он нужен!!!)

8.5.3 Fundamentals of Inelastic Collisions

(тут большая теория, в том числе в ЛЛ3, потом напишу)

Неупругие столкновения

При изложении фазовой теории рассеяния мы полагали, что поток вероятности сохраняется: число падающих на мишень частиц равно числу рассеянных, так что имеет место тождество

$$|S_l| \equiv 1$$

и рассеяние происходит упругим образом.

Однако, если в процессе столкновения образуются частицы, отличные от исходных, то говорят, что открываются неупругие каналы рассеяния: пространство асимптотических состояний двух частиц становится неполным, часть падающего потока инициирует неупругие процессы, и

$$|S_l| < 1$$

Тогда сечение упругих (elastic) столкновений с $f_l = (2l+1)(S_l - 1)/(2\mathrm{i}k)$

$$\sigma_{\mathrm{el}} = \frac{\pi}{k^2}\sum_l (2l+1)\,|S_l - 1|^2$$

а недостающий поток вероятности в рассеянной волне, пропорциональный $1 - |S_l|^2$, естественно отнести к сечению неупругих (inelastic) столкновений, так что его полное сечение

$$\sigma_{\mathrm{inel.}} = \frac{\pi}{k^2}\sum_l (2l+1)\left(1 - |S_l|^2\right)$$

Полное (total) сечение

$$\sigma_{\mathrm{tot.}} = \sigma_{\mathrm{el.}} + \sigma_{\mathrm{inel.}} = \frac{\pi}{k^2}\sum_l (2l+1)\left\{|S_l - 1|^2 + 1 - |S_l|^2\right\}$$

Преобразуем

$$|S_l - 1|^2 + 1 - |S_l|^2 = (S_l - 1)(S_l^* - 1) + 1 - |S_l|^2 = 2 - (S_l + S_l^*) = 2\,(1 - \mathrm{Re}_\ell S_l)$$

В итоге

$$\sigma_{\mathrm{tot.}} = \frac{2\pi}{k^2}\sum_l (2l+1)\,(1 - \mathrm{Re}eS_l)$$

Заметим, что

$$\mathrm{Im}\mathfrak{m} f_l = \frac{2l+1}{2k}\mathrm{Im}\mathfrak{m}\frac{1}{i}\left(\mathrm{Re}_{\mathfrak{e}} S_l - 1 + \mathrm{i}\mathrm{Im}\mathfrak{m} S_l\right) = \frac{2l+1}{2k}\left(1 - \mathrm{Re}_e S_l\right)$$

тогда по прежнему справедлива оптическая теорема

$$\sigma_{\mathrm{tot.}} = \frac{4\pi}{k}\sum_l \mathrm{Im}m f_l$$

Что отражает факт сохранения вероятности с учетом вклада неупругих столкновений.

8.5.4 Second order Born approximation (??)

(see articles for now!)

Formalism of second order Born approximation

Examples of second order Born approximation

Details of second order Born approximation

8.5.5 Reconstruction of the potential from scattering

(??? currently have no idea how to do it)

8.5.6 Time Delay in Scattering

(тоже инетерсно, как ее посчитать?)

8.5.7 Quantum mechanics of the $1/x^2$ potential by Essin, Griffiths (2005) 1

Abstract

In quantum mechanics a localized attractive potential typically supports a (possibly infinite) set of bound states, characterized by a discrete spectrum of allowed energies, together with a continuum of scattering states, characterized (in one dimension) by an energy-dependent phase shift. The $1/x^2$ potential on $0 < x < \infty$ confounds all of our intuitions and expectations. Resolving its paradoxes requires sophisticated theoretical machinery: regularization, renormalization, anomalous symmetry-breaking, and self-adjoint extensions. Our goal is to introduce the essential ideas at a level accessible to advanced undergraduates. © 2006 American Association of Physics Teachers.

I. INTRODUCTION

Ordinarily, an attractive potential admits discrete bound states, together (perhaps) with a continuum of scattering states. In a first course on quantum mechanics, students encounter the infinite square well, the harmonic oscillator, the Dirac delta function, the finite square well, and (in three dimensions) the spherical well and the Coulomb potential, all of which fit this paradigm (though the first two lack scattering states). We do not study the $1/x^2$ potential, and for good reason: It violates every rule in the book, and discredits all the intuition we are trying to instill in our students. In spite of this (or rather, precisely because of it) the $1/x^2$ potential is a fascinating system, and analyzing its paradoxes provides an illuminating introduction to some of the more subtle techniques in contemporary theoretical physics: regularization and renormalization, anomalous symmetry-breaking, and self-adjoint extensions. In this paper we tell the story from a pedagogical perspective, starting out innocent and naive, and letting the unfolding saga force us to become wiser and more sophisticated.

In Sec. II we introduce the problem in its simplest (onedimensional) form, and approach it as we would any other quantum system. We quickly encounter a series of puzzles and surprises. In Sec. III we identify the source of the difficulties and modify the potential so as to avoid the trouble. This leads naturally to renormalization and anomalies. In Sec. IV we notice that the Hamiltonian is not Hermitian, and modify the space of permissible functions to make it so; this introduces the method of self-adjoint extensions. In Sec. V we draw lessons from our experience and point to some realworld applications.

II. PECULIARITIES OF THE $1/x^2$ POTENTIAL

Consider a particle of mass m in the one-dimensional potential [1]

$$V(x) = \begin{cases} \infty & (x \leqslant 0) \\ -a/x^2 & (x > 0) \end{cases} \tag{1}$$

shown in Fig. 1. Here a is a constant with the (MKS) units Jm^2. In truth, the alarm should already be sounding, for there is no way to construct a quantity with the dimensions of energy from the parameters at hand ($\hbar, m$, and a), and hence no possible formula for the eigenvalues of the

Hamiltonian. [2] But let's pretend for a moment that we did not notice this problem. We look for bound states-normalizable negative-energy solutions of the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \frac{a}{x^2}\psi = E\psi \quad (x > 0) \tag{2}$$

or, multiplying through by $-2m/\hbar^2$,

$$\frac{d^2\psi}{dx^2} + \frac{\alpha}{x^2}\psi = \kappa^2\psi, \tag{3}$$

where $\alpha \equiv 2ma/\hbar^2$ and $\kappa \equiv \sqrt{-2mE}/\hbar$, subject to the boundary conditions

$$\psi \to 0 \text{ as } x \to 0 \text{ and } x \to \infty. \tag{4}$$

The first boundary condition is necessary to make ψ continuous at the origin ($\psi = 0$, of course, for $x < 0$); the second is required for normalization:

$$\int_0^\infty |\psi(x)|^2 dx = 1 \tag{5}$$

Suppose we could find just one bound state $\psi(x)$, with energy E. Scaling x by a factor β, we can immediately construct a new solution, $\psi_\beta(x) \equiv \psi(\beta x)$, with energy $\beta^2 E$:

$$\begin{aligned}\frac{d^2\psi_\beta}{dx^2} + \frac{\alpha}{x^2}\psi_\beta =& \frac{d^2}{dx^2}\psi(\beta x) + \frac{\alpha}{x^2}\psi(\beta x) = \beta^2\frac{d^2}{du^2}\psi(u) \\ &+ \beta^2\frac{\alpha}{u^2}\psi(u) = \beta^2\kappa^2\psi(u) = (\beta\kappa)^2\psi_\beta(x)\end{aligned} \tag{6}$$

where $u \equiv \beta x$. But β can be any real number. [3] So if there exist any bound states, then there is a bound state for every negative energy! In particular, the $1/x^2$ potential has no ground state. This is disturbing, for a system without a lower limit on its allowed energies would be wildly unstable, cascading down with the release of an unlimited amount of energy. A reasonable inference would be that there are no negative energy states, which is indeed the case for $\alpha < 1/4$ (trivially so, for $\alpha < 0$, because the potential is then repulsive).

Fig. 1. The $1/x^2$ potential.

One particularly nice way to show that there are no bound states for $0 < \alpha < 1/4$ is to factor the Hamiltonian. [4] Let $\alpha = \nu(1-\nu)$ define the new constant ν,

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \frac{a}{x^2} = -\frac{\hbar^2}{2m}\left(\frac{d}{dx} + \frac{\nu}{x}\right)\left(\frac{d}{dx} - \frac{\nu}{x}\right). \tag{7}$$

For an arbitrary test function $f(x)$ we have

$$\left(\frac{d}{dx} + \frac{\nu}{x}\right)\left(\frac{d}{dx} - \frac{\nu}{x}\right)f(x) = \left(\frac{d}{dx} + \frac{\nu}{x}\right)\left(\frac{df}{dx} - \frac{\nu}{x}f\right) \tag{8a}$$

$$= \frac{d^2f}{dx^2} + \frac{\nu}{x^2}f - \frac{\nu}{x}\frac{df}{dx} + \frac{\nu}{x}\frac{df}{dx} - \frac{\nu^2}{x^2}f \tag{8b}$$

$$= \frac{d^2f}{dx^2} + \frac{\nu(1-\nu)}{x^2}f = \left(\frac{d^2}{dx^2} + \frac{\alpha}{x^2}\right)f \tag{8c}$$

Now, the Hermitian conjugate of $(d/dx + \nu/x)$ is $(-d/dx\ + \nu^*/x)$:

$$\left\langle f \left| \left(\frac{d}{dx} + \frac{\nu}{x}\right) g \right\rangle = \int_0^\infty f^* \left(\frac{dg}{dx} + \frac{\nu}{x} g\right) dx \tag{9a}$$

$$= f^* g|_0^\infty - \int_0^\infty \left(\frac{df}{dx}\right)^* g dx + \int_0^\infty \left(\frac{\nu^*}{x} f\right)^* g dx \tag{9b}$$

$$= \left\langle \left(-\frac{d}{dx} + \frac{\nu^*}{x}\right) f \right| g \right\rangle, \tag{9c}$$

provided that $f(x)$ and $g(x)$ go to zero at 0 and ∞. Thus

$$E = \langle H \rangle = \langle \psi | H | \psi \rangle = -\frac{\hbar^2}{2m} \left\langle \psi \left| \left(\frac{d}{dx} + \frac{\nu}{x}\right) \left(\frac{d}{dx} - \frac{\nu}{x}\right) \psi \right\rangle \right. \tag{10a}$$

$$= \frac{\hbar^2}{2m} \left\langle \left(\frac{d}{dx} - \frac{\nu^*}{x}\right) \psi \right| \left(\frac{d}{dx} - \frac{\nu}{x}\right) \psi \right\rangle. \tag{10b}$$

If ν is real, then,

$$E = \frac{\hbar^2}{2m} \int_0^\infty \left| \left(\frac{d\psi}{dx} - \frac{\nu}{x}\psi\right) \right|^2 dx > 0 \tag{11}$$

so negative energy states cannot occur if ν is real. But $\nu(1 - \nu) = \alpha$, so

$$\nu = \frac{1}{2} \pm \sqrt{\frac{1}{4} - \alpha}, \tag{12}$$

and hence if $\alpha < 1/4$, then ν is real, and there can be no bound states.

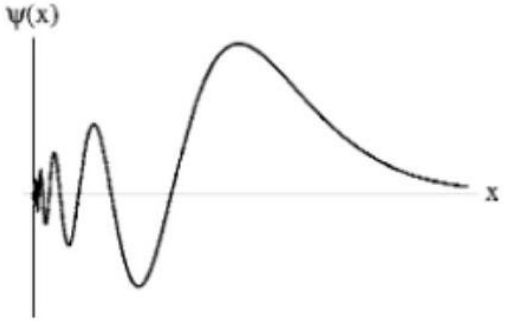


Fig. 2. The bound state wave function, $\psi_\kappa(x)$.

But when $\alpha > 1/4$ there certainly do exist negative energy solutions. The Schrödinger equation can be solved by the method of Frobenius: We write $\psi(x)$ as a power series,

$$\psi(x) = x^s \sum_{j=0}^\infty a_j x^j \quad (a_0 \neq 0) \tag{13}$$

and substitute this into Eq. (3):

$$\sum_{j=0}^\infty a_j [(j+s)(j+s-1) + \alpha] x^{j-2} = \kappa^2 \sum_{j=0}^\infty a_j x^j \tag{14}$$

We equate like powers and find that the x^{-2} term yields $s(s\ -1) + \alpha = 0$, so

$$s = \nu = (1/2) \pm \sqrt{(1/4) - \alpha} \tag{15}$$

the x^{-1} term forces $a_1 = 0$, and the remaining coefficients are determined by the recursion relation

$$a_j = \frac{\kappa^2}{j(j+2s-1)} a_{j-2} \quad (j = 2, 3, 4, ...) \tag{16}$$

There are two solutions-one for each sign in Eq. (15). Near the origin they go like $a_0 x^s$; for $\alpha > 1/4$ this means

$$\sqrt{x} e^{\pm ig \ln x} \tag{17}$$

where $g \equiv \sqrt{\alpha - 1/4}$.
The general solution is a linear combination, but it turns out that only one combination is normalizable:

$$\psi_\kappa(x) = A\sqrt{x} K_{ig}(\kappa x) \tag{18}$$

where K_{ig} is the modified Bessel function of order ig;[5] ψ_κ is real, as long as g is real (which is to say, for $\alpha > 1/4$), and finite at the origin (so $\psi_\kappa \to 0$ as $x \to 0$); ψ_κ itself is square-integrable: [(1)]

$$\int_0^\infty \left|\sqrt{x} K_{ig}(\kappa x)\right|^2 dx = \frac{\pi g}{2\kappa^2 \sinh(\pi g)} \tag{19}$$

so the normalization constant is

$$A = \kappa \sqrt{\frac{2\sinh(\pi g)}{\pi g}} \tag{20}$$

A plot of the wave function is shown in Fig. 2. Notice the oscillations as $x \to 0$, which result from the sinusoidal dependence on $g \ln x$ in Eq. (17). We are accustomed to the idea that the ground state has no zero crossings, the first excited state has one, the second two, and so on. But the $1/x^2$ potential has no ground state, and every (negative energy) solution has an infinite number of zero crossings. If the number of nodes counts the number of lower energy states, then no matter what the energy, there are always infinitely many states even lower.

What about positive energy (scattering) states? For $E > 0$ the general solution to Schrödinger's equation [Eq. (2)] is

$$\psi_k(x) = \sqrt{x}\left[A H_{ig}^{(2)}(kx) + B H_{ig}^{(1)}(kx)\right], \tag{21}$$

where $k \equiv \sqrt{2mE}/\hbar$, and $H^{(1)}$ and $H^{(2)}$ are Hankel functions. For large x, [8]

$$H_{ig}^{(1)}(kx) \sim \sqrt{\frac{2}{\pi kx}} e^{i(kx - \pi/4)} e^{\pi g/2} \tag{22a}$$

$$H_{ig}^{(2)}(kx) \sim \sqrt{\frac{2}{\pi kx}} e^{-i(kx - \pi/4)} e^{-\pi g/2} \tag{22b}$$

so

$$\psi_k(x) \sim A\sqrt{\frac{2}{\pi k}} e^{-\pi g/2} e^{i\pi/4}\left[e^{-ikx} - i\frac{B}{A} e^{\pi g} e^{ikx}\right] \tag{23}$$

The first term (e^{-ikx}) represents a wave incident from the right; the second $\left(e^{ikx}\right)$ is the reflected wave. Ordinarily, setting $\psi_k(0) = 0$ in Eq. (21) would determine B/A, and the asymptotic expression Eq. (23) would reduce to [9]

$$\psi_k(x) \sim \left[e^{-ikx} - e^{i(2\delta+kx)}\right] \tag{24}$$

indicating that the reflected wave is equal in amplitude to the incident wave (as required by conservation of probability) and shifted in phase by an amount $\delta(k)$. But in this case $\psi_k(0)$ is automatically zero (according to Eq. (17), $|\psi| \sim \sqrt{x}$). There is no constraint on B, no formula for $\delta(k)$, and (most alarming) no enforcement of conservation of probability; the outgoing wave can have any amplitude!

Conclusion: The $1/x^2$ potential has no ground state, and the allowed energies are not quantized. As long as $\alpha > 1/4$, the Schrödinger equation can be solved (and the boundary conditions satisfied) for every negative energy; the solutions are real and normalizable, and each of them has an infinite number of zero crossings. Scattering states occur for every positive energy, but the boundary condition at $x = 0$ imposes no constraint on the reflection coefficient, and does not determine the phase shift. It would be difficult to imagine a situation more at odds with our expectations.

III. REGULARIZATION, RENORMALIZATION, AND ANOMALIES

Physically, the $1/x^2$ potential is just too strong at the origin- $1/x$ is acceptable, [10] but $1/x^2$ is not. One way to avoid the problem is to move the "wall" over to the right a distance ϵ:

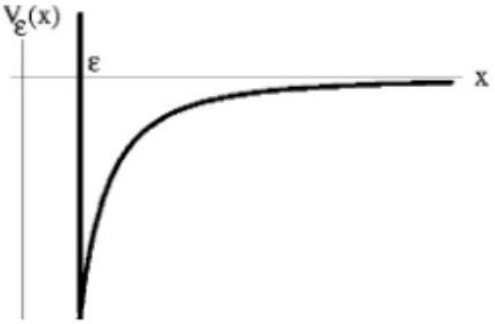


Fig. 3. The regularized potential.

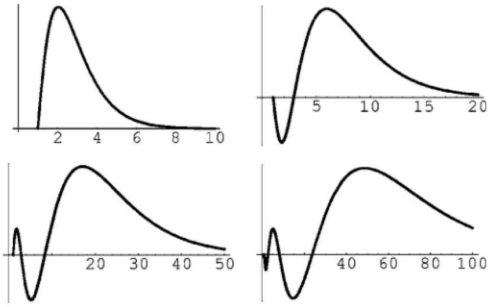


Fig. 4. Ground state and first three excited states, as functions of κx, for V_ϵ, with $\epsilon = 1$ and $g = 3$ (not normalized).

$$V_\epsilon(x) = \begin{cases} \infty & (x \leqslant \epsilon) \\ -a/x^2 & (x > \epsilon), \end{cases} \tag{25}$$

as shown in Fig. 3. This "regularized" potential suffers none of the ills that afflict $V(x)$; we propose to work with $V_\epsilon(x)$, and take the limit $\epsilon \to 0$ only at the very end. Of course, the pathologies can be expected to reappear in this limit, but as we shall see, some predictions survive, and these we take to be the "true" physical content of the $1/x^2$ system. This is the strategy of "renormalization."

Having introduced a parameter (ϵ) with the units of length, we are now able to construct an expression with the dimensions of energy:

$$\frac{a}{\epsilon^2} f(\alpha) \tag{26}$$

where f is a function of the dimensionless quantity $\alpha = 2ma/\hbar^2$. The system is no longer scale invariant; it possesses both a ground state [11] and a discrete spectrum of bound states. These have the same functional form as in Eq. (18), but the boundary condition is now $\psi_\kappa(\epsilon) = 0$, which implies that

$$K_{ig}(\kappa\epsilon) = 0 \tag{27}$$

which is not automatically satisfied, and serves to quantize the energy. Figure 4 shows the ground state and the first three excited states for the case $\alpha = 9.25 (g = 3)$.[12] Figure 5 shows the ground state energy (or rather, $\kappa_1\epsilon$) for g ranging up to 7 .

If $\kappa\epsilon \ll 1$, [13] we can provide a relatively simple formula for the allowed energies: [14]

$$K_{ig}(z) \approx -\sqrt{\frac{\pi}{g\sinh(\pi g)}} \times \sin\left[g\ln\left(\frac{z}{2}\right) - \arg\Gamma(1+ig)\right] \quad (z \ll 1) \tag{28}$$

so $K_{ig}(\kappa\epsilon) = 0$ implies

$$g\ln\left(\frac{\kappa\epsilon}{2}\right) - \arg\Gamma(1+ig) + n\pi = 0 \tag{29}$$

where n is an integer. The ground state is $n = 1$, [15] and the excited states are $n = 2, 3, ...$, with

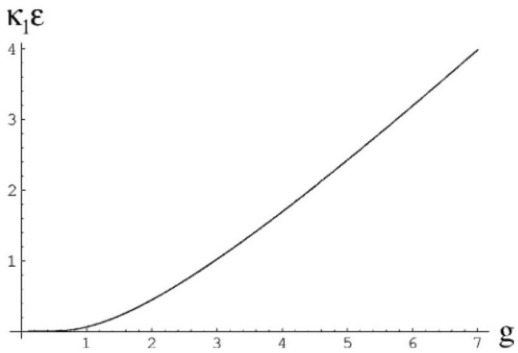


Fig. 5. The ground state $\kappa_1\epsilon$ as a function of g.

$$\kappa_n = \frac{2}{\epsilon} e^{[\arg\Gamma(1+ig) - n\pi]/g}, \tag{30}$$

or

$$E_n = -\frac{2\hbar^2}{m\epsilon^2} e^{2[\arg\Gamma(1+ig) - n\pi]/g} \tag{31}$$

There are infinitely many discrete bound states, as one might expect. [16]

For positive energies (scattering) the wave function is still given by Eq. (21), but now

$$\psi_k(\epsilon) = 0, \tag{32}$$

and hence $AH_{ig}^{(2)}(k\epsilon) + BH_{ig}^{(1)}(k\epsilon) = 0$, so

$$\frac{B}{A} = -\frac{H_{ig}^{(2)}(k\epsilon)}{H_{ig}^{(1)}(k\epsilon)}. \tag{33}$$

Referring to Eqs. (23) and (24), we find that the phase shift satisfies [P]

$$e^{2i\delta} = i\frac{B}{A}e^{\pi g} = -i\frac{H_{ig}^{(2)}(k\epsilon)}{H_{ig}^{(1)}(k\epsilon)}e^{\pi g} = -i\frac{\left[H_{ig}^{(1)}(k\epsilon)\right]^*}{H_{ig}^{(1)}(k\epsilon)}. \tag{34}$$

Notice that conservation of probability has been enforced by Eq. (32). Thus

$$\delta = -\arg\left[H_{ig}^{(1)}(k\epsilon)\right] - \frac{\pi}{4}. \tag{35}$$

This function is plotted in Fig. 6.
As the graphs suggest, $\arg\left[H_{ig}^{(1)}(x)\right]$ is extremely steep near the origin. Indeed, for $|z| \ll 1$, [18]

$$H_{ig}^{(1)}(z) \approx e^{ig\ln(z/2)}\frac{1+\coth\pi g}{\Gamma(1+ig)} - e^{-ig\ln(z/2)}\frac{\Gamma(1+ig)}{\pi g}, \tag{36}$$

so [19]

$$\tan\left[\arg H_{ig}^{(1)}(z)\right] \approx \coth\left(\frac{\pi g}{2}\right) \times \tan[g\ln(z/2) - \arg\Gamma(1+ig)] \tag{37}$$

and hence

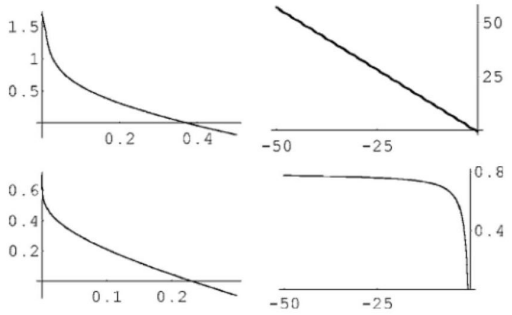


Fig. 6. Graphs of δ as a function of $k\epsilon$, for $g = 0.5$ (top) and $g = 0$ (bottom). The graphs on the right show the behavior near the origin (the horizontal scale is in powers of 10); they suggest that there is no limit when $g = 0.5$, whereas $\delta \to \pi/4$ when $g = 0$ (though that limit is only approached when $k \in \ll 10^{-10}$).

$$\tan\delta \approx \frac{\tan\xi + \tanh(\pi g/2)}{\tan\xi - \tanh(\pi g/2)}, \tag{38}$$

where

$$\xi \equiv g\ln(k\epsilon/2) - \arg\Gamma(1+ig). \tag{39}$$

As $k\epsilon \to 0, \xi \to -\infty$, and $\tan\xi$ fluctuates wildly: Whenever ξ hits an integer multiple of π, $\tan\xi = 0$, so (unless $g = 0$) $\tan\delta = -1$; whenever ξ is a half-integer multiple of $\pi, \tan\xi \to \pm\infty$, so $\tan\delta = 1$. Clearly, δ does not approach a limit. The case $g = 0$ is special, and it is best to treat it separately: For $|z| \ll 1$,

$$H_0^{(1)}(z) \approx 1 + \frac{2i}{\pi}[\ln(z/2) + C] = 1 + \frac{2i}{\pi}\ln(\gamma z/2), \tag{40}$$

where $C = 0.577215$ is Euler's constant and $\gamma \equiv e^C = 1.781072$.[20] Thus $\tan\left[\arg H_0^{(1)}(z)\right] \approx 2\ln(\gamma z/2)/\pi$, and hence

$$\tan\delta \approx \frac{\ln(\gamma k\epsilon/2)+\pi/2}{\ln(\gamma k\epsilon/2)-\pi/2} \tag{41}$$

At this point we would like to send $\epsilon \to 0$, to recover the pure $1/x^2$ potential. Naively, Eq. (31) suggests that E_1 will go to $-\infty$-precisely the trap we were hoping to avoid. But closer inspection reveals that the boundary condition, Eq. (27), only determines the product $\kappa_1\epsilon$. Suppose we stipulate that E_1 (and hence κ_1) remain constant as $\epsilon \to 0$. From Fig. 5 we see that this assumption forces $g \to 0$, leaving [16]

$$\kappa_1 = \frac{2}{\gamma\epsilon}e^{-\pi/g} \quad (\epsilon \to 0, g \to 0). \tag{42}$$

The excited states, Eq. (30), are squeezed out

$$\kappa_n = \frac{2}{\gamma\epsilon}e^{-n\pi/g} = \kappa_1 e^{-(n-1)\pi/g} \to 0 \quad (n = 2, 3, 4, ...), \tag{43}$$

but there remains a single bound state at finite (though indeterminate) energy.

We can use Eq. (42) to eliminate the cutoff ϵ in favor of κ_1, in the scattering problem:

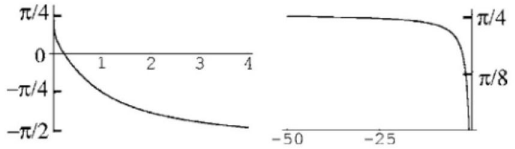


Fig. 7. The scattering phase shift $\delta(k/\kappa_1)$, Eq. (47), for $g \ll 1$. The graph on the right shows the behavior near the origin (the horizontal scale is in powers of 10).

$$k\epsilon = \frac{k}{\kappa_1}\frac{2}{\gamma}e^{-\pi/g}. \tag{44}$$

So for low energy scattering, Eq. (39) becomes

$$\xi \approx g\ln(k/\kappa_1) - \pi \tag{45}$$

$$\tan\xi \approx \tan[g\ln(k/\kappa_1)] \approx g\ln(k/\kappa_1) \tag{46}$$

and Eq. (38) reads

$$\tan\delta \approx \frac{\ln(k/\kappa_1)+\pi/2}{\ln(k/\kappa_1)-\pi/2} \tag{47}$$

Curiously, the phase shift is independent of g (although we have stipulated that $g \ll 1$). [21] For extremely low-energy scattering, $k \ll \kappa_1$, the phase shift is evidently $\pi/4$ (see Fig. 7).

Conclusion: The regularized potential, Eq. (25), has a nonproblematic spectrum of discrete bound states, and a continuum of scattering states with well-defined phase shifts. Naively, the limit $\epsilon \to 0$ (which restores the pure $1/x^2$ potential) reintroduces all of the pathological features of the original. But closer examination reveals a loophole: If as we send $\epsilon \to 0$ we simultaneously let $g \to 0$, in such a way as to hold κ_1 constant (Fig. 8), then a single bound state with energy

$$E_1 = -\frac{\hbar^2\kappa_1^2}{2m} \tag{48}$$

survives, and the scattering phase shift is given by

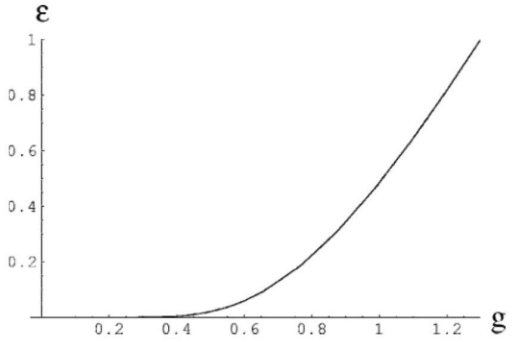


Fig. 8. Graph of ϵ as a function of g, Eq. (42), with $\kappa_1 = 0.1$.

$$\delta(k) = \tan^{-1}\left[\frac{\ln(k/\kappa_1) + \pi/2}{\ln(k/\kappa_1) - \pi/2}\right] \tag{49}$$

This scheme does not determine κ_1, and it forces $\alpha \to 1/4$, but the physical implications of the theory are perfectly sensible.

The renormalization procedure we have just described may sound artificial, but it is not altogether unreasonable. [22] After all, in practice we would have no way of knowing whether the potential is really $1/x^2$ all the way down to $x = 0$; what we actually measure is the ground state energy and the scattering phase shift. The former provides us with a relation between ϵ and g, Eq. (42), but it does not determine either one separately, and the latter, Eq. (49), stands as a testable prediction irrespective of the actual (but unmeasurable) value of the cutoff. [23]

What about the symmetry argument based on scale invariance (or, if you prefer, dimensional analysis) that seemed to prove conclusively that the $1/x^2$ potential can have no ground state (if it has one negative allowed energy, then every negative energy is an eigenvalue)? Well, we broke that symmetry when we introduced the cutoff, and the break persists even as we eliminate ϵ from the theory in favor of κ_1, and (implicitly) send $\epsilon \to 0$. This is an example of "anomalous" symmetry breaking. There are three standard mechanisms for breaking a symmetry in physics:

1. External (or dynamical): An imposed force spoils the symmetry (for example, at the surface of the earth gravity breaks the three-dimensional isotropy of space).

2. Spontaneous: The ground state of a system is degenerate, and historical accident selects a particular one (for example, the magnetization of a small piece of iron, which could have pointed in any direction, but in fact has to point in some specific direction).

3. Anomalies: The process of renormalization breaks the symmetry. [24]

8.5.8 Quantum mechanics of the $1/x^2$ potential by Essin, Griffiths (2005) 2

IV. SELF-ADJOINT EXTENSIONS

In Sec. II we examined the patient and diagnosed the illness. In Sec. III we provided a partial cure. Now it is time to identify the root cause of the disease and propose a more comprehensive treatment. The fundamental problem with the $1/x^2$ potential is that the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \frac{a}{x^2} = -\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2} + \frac{\alpha}{x^2}\right) \tag{50}$$

is not Hermitian (more precisely, it is not self-adjoint). In quantum mechanics self-adjoint operators occupy a privileged position, because they alone represent observable quantities.

Most of our experience and intuition is predicated on the self-adjointness of the Hamiltonian, and when this fails, the intelligibility of the theory goes with it.

An operator is defined not only by its action, A, but also by its domain, $\mathcal{D}_A$, the space of functions $\{\psi\}$ on which it acts. Physicists tend to forget the second part, because in most cases the domain is not problematic. Of course, ψ and $A\psi$ must lie in the Hilbert space of square-integrable functions, L_2 (in our case, on the interval $0 < x < \infty$), to ensure that inner products are well-defined. In fact, to guarantee the existence of the Hermitian conjugate (or "adjoint") $A^\dagger$,

$$\langle \phi | A\psi \rangle = \left\langle A^\dagger \phi | \psi \right\rangle, \tag{51}$$

the allowed functions must be dense in L_2.[25] Typically there will be other conditions on $\mathcal{D}_A$ as well.

If there exists a domain such that for all ψ and ϕ in $\mathcal{D}_A$

$$\langle \phi | A\psi \rangle = \langle A\phi | \psi \rangle \tag{52}$$

(that is, the actions of A and $A^\dagger$ are identical), then the operator is Hermitian (mathematicians would say "symmetric") over that domain. However, it may happen that as long as ψ is in $\mathcal{D}_A$ (the domain of the operator), ϕ can be in a larger domain, $\mathcal{D}_{A^\dagger}$ (the domain of the adjoint), [26] and yet Eq. (52) still holds. In that case ($\mathcal{D}_{A^*} \supset \mathcal{D}_A$) we may be able to extend the domain of the operator (which will automatically restrict the domain of the adjoint) until the two domains coincide. In this circumstance, with $A = A^\dagger$ and $\mathcal{D}_{A^\dagger} = \mathcal{D}_A$, the operator is said to be self-adjoint. For self-adjoint operators, in other words, both the action and the domain of the adjoint are the same as for the operator itself.

The process we have sketched is called "self-adjoint extension." You start with a Hermitian operator on a specified domain, and extend $\mathcal{D}_A$ (thereby contracting $\mathcal{D}_{A^\dagger}$) until the domains are identical. This process raises several questions, which were first addressed by Weyl and later generalized by von Neumann and Stone: [27] How can you tell whether a given operator admits a self-adjoint extension? Is the extension (if it exists) unique? How do you construct the self-adjoint domain? The answers are buried in abstruse mathematical literature that is largely inaccessible to physicists, [28] but two recent articles provide a relatively straightforward guide for the uninitiated. [29,30]

We begin by asking whether H in Eq. (50) is Hermitian. Suppose $\phi(x)$ and $\psi(x)$ are two functions in $L_2(0,\infty)$ such that $H\phi$ and $H\psi$ are also in $L_2(0,\infty)$. Using integration by parts (twice), we have

$$\langle \phi | H\psi \rangle = \frac{-\hbar^2}{2m} \int_0^\infty \phi^* \left(\frac{d^2\psi}{dx^2} + \frac{\alpha}{x^2}\psi \right) dx \tag{53a}$$

$$= -\frac{\hbar^2}{2m} \left[\phi^* \frac{d\psi}{dx}\bigg|_0^\infty - \psi \frac{d\phi^*}{dx}\bigg|_0^\infty + \int_0^\infty \left(\frac{d^2\phi^*}{dx^2} + \frac{\alpha}{x^2}\phi^* \right) \psi dx \right] \tag{53b}$$

$$= \langle H\phi | \psi \rangle - \frac{\hbar^2}{2m} \left(\phi^* \frac{d\psi}{dx} - \psi \frac{d\phi^*}{dx} \right) \bigg|_0^\infty \tag{53c}$$

Evidently H is Hermitian,

$$\langle \phi | H\psi \rangle = \langle H\phi | \psi \rangle, \tag{54}$$

if the boundary term in Eq. (53c) is zero (for all ψ and ϕ). There is no problem at infinity, where the functions and their derivatives can safely be taken to vanish; [31] the trouble arises at the lower limit. If we want H to be Hermitian, we shall have to restrict its domain. Earlier, we

stipulated (for reasons of continuity) that wave functions go to zero at the origin, but in spite of appearances this condition does not suffice to kill the boundary term, because the derivatives can (and in the critical cases do) diverge. For example, we found in Eq. (15) that solutions to the Schrödinger equation behave near the origin like

$$u_\pm(x) = x^{S_\pm} \tag{55a}$$

with

$$s_\pm = \frac{1}{2} \pm \sqrt{\frac{1}{4} - \alpha} \tag{55b}$$

So, using $\psi = u_+$and $\phi = u_-$, we have [32]

$$\begin{aligned}\left(u_-^* \frac{du_+}{dx} - u_+ \frac{du_-^*}{dx}\right)\Big|_0 &= x^{(s_-)^*} s_+ x^{(s_+-1)} - x^{s_+} s_-^* x^{\left(s_-^*-1\right)} \\ &= \left(s_+ - s_-^*\right) x^{\left(s_++s_-^*-1\right)} = \sqrt{1-4\alpha}\end{aligned} \tag{56}$$

Unless $\alpha = 1/4$ (a special case that keeps recurring and to which we shall return) some other condition must be imposed.

What if we insist that allowed functions vanish in a finite (but arbitrarily small) neighborhood [33] of the origin? Then the boundary term vanishes trivially, and H is Hermitian (on this domain). But if ψ is in this very restricted domain, ϕ could be any square-integrable function, and the boundary term will still vanish. So the domain of the adjoint is very much larger than the domain of the operator, and hence H is not self-adjoint. Question: Does H admit a self-adjoint extension, and if so, what is the self-adjoint domain? [34] In von Neumann's procedure the first step is to look for eigenfunctions of H with imaginary eigenvalues: [35]

$$H\phi_\pm = \pm i\eta\phi_\pm, \tag{57}$$

where η is real and positive. [36] Thus

$$\left(\frac{d^2}{dx^2} + \frac{\alpha}{x^2}\right)\phi_\pm = \kappa_\pm^2 \phi_\pm \tag{58}$$

where

$$\kappa_\pm \equiv \frac{\sqrt{\mp i 2m\eta}}{\hbar} = e^{\mp i\pi/4}\beta \tag{59}$$

with $\beta \equiv \sqrt{2m\eta}/\hbar$. The general solution is

$$\phi_\pm(x) = \sqrt{x}\left[A_\pm H_{ig}^{(1)}\left(i\kappa_\pm x\right) + B_\pm H_{ig}^{(2)}\left(i\kappa_\pm x\right)\right] \tag{60}$$

where (as always) $g = \sqrt{\alpha - 1/4}$, and $A_\pm$and $B_\pm$are arbitrary constants. But $H_{ig}^{(2)}\left(i\kappa_\pm x\right)$ is not in L_2 (and hence not in $\mathcal{D}_{H^\dagger}$), because at large x [Eq. (22b)][37]

$$\begin{aligned}H_{ig}^{(2)}\left(i\kappa_\pm x\right) &\approx \sqrt{\frac{2}{\pi i\kappa_\pm x}} e^{-i(i\kappa_\pm x - \pi/4)} e^{-\pi g/2} \\ &= \sqrt{\frac{2}{\pi\kappa_\pm x}} e^{-\pi g/2} e^{\kappa_\pm x}\end{aligned} \tag{61}$$

and because $\kappa = \beta(1 \mp i)/\sqrt{2}, H_{ig}^{(2)}$ diverges exponentially. Thus

$$\phi_{\pm}(x) = A_{\pm}\sqrt{x}H_{ig}^{(1)}\left(i\kappa_{\pm}x\right) \tag{62}$$

Let n_+be the number of linearly independent solutions for ϕ_+, and $n_-$the corresponding number for ϕ_-; n_1 and n_2 are called "deficiency indices," and they play a major role in the theory. Weyl and von Neumann showed that if $n_+ = n_- = n$, there exists an n^2-parameter family of self-adjoint extensions. (If $n = 0$, the operator is already self-adjoint, and if $n_+ \neq n_-$, there is no self-adjoint extension.) In our case, n_+
$= n_- = 1$, and it remains only to characterize the oneparameter family of self-adjoint domains. The prescription is as follows: ψ is in the self-adjoint domain if

$$\langle\Phi|H\psi\rangle = \langle H\Phi|\psi\rangle, \tag{63}$$

where $\Phi \equiv \phi_+ + \lambda\phi_-$for some λ, which is to say [Eq. (53c)] if

$$\lim_{x\to 0}\left[\Phi^*\frac{d\psi}{dx} - \psi\frac{d\Phi^*}{dx}\right] = 0 \tag{64}$$

Evidently we need to know the behavior of $\phi_{\pm}$for small x. From Eq. (36),

$$\begin{aligned} H_{ig}^{(1)}\left(i\kappa_{\pm}x\right) \approx & e^{ig\ln(i\kappa_{\pm}x/2)}\frac{1+\coth\pi g}{\Gamma(1+ig)} \\ & - e^{-ig\ln(i\kappa_{\pm}x/2)}\frac{\Gamma(1+ig)}{\pi g} \end{aligned} \tag{65}$$

provided that $g \neq 0$. But $\kappa_{\pm} = \exp(\mp i\pi/4)\beta$, so

$$\ln\left(i\kappa_{\pm}x/2\right) = \ln(\beta x) - \ln 2 + i\ell_{\pm}\pi/4, \tag{66}$$

where $\ell_+ \equiv 1$ and $\ell_- \equiv 3$. Thus

$$e^{ig\ln(i\kappa_{\pm}x/2)} = e^{ig\ln\beta x}e^{-ig\ln 2}e^{-\ell_{\pm}g\pi/4} \tag{67}$$

and hence

$$\phi_+ \approx A_+\sqrt{x}\left[De^{ig\ln\beta x} - Fe^{-ig\ln\beta x}\right], \tag{68a}$$

$$\phi_- \approx A_-\sqrt{x}\left[De^{-\pi g/2}e^{ig\ln\beta x} - Fe^{\pi g/2}e^{-ig\ln\beta x}\right], \tag{68b}$$

where

$$D \equiv e^{-ig\ln 2}e^{-\pi g/4}\left[\frac{1+\coth\pi g}{\Gamma(1+ig)}\right], \tag{69a}$$

$$F \equiv e^{ig\ln 2}e^{\pi g/4}\left[\frac{\Gamma(1+ig)}{\pi g}\right]. \tag{69b}$$

It follows that

$$\Phi \approx \sqrt{x}\left[Ge^{ig\ln\beta x} - Je^{-ig\ln\beta x}\right] \quad (x \ll 1), \tag{70}$$

where

$$G \equiv D\left(A_+ + \lambda A_- e^{-\pi g/2}\right) \tag{71a}$$

$$J \equiv F\left(A_+ + \lambda A_- e^{\pi g/2}\right) \tag{71b}$$

Therefore

$$\frac{d\Phi}{dx} \approx \frac{1}{\sqrt{x}}\left[\left(\frac{1}{2}+ig\right)Ge^{ig\ln\beta x} - \left(\frac{1}{2}-ig\right)Je^{-ig\ln\beta x}\right]. \tag{72}$$

Using Eqs. (70) and (72), the boundary condition [Eq. (64), or more simply its complex conjugate] becomes

$$\sqrt{x}\left[e^{2ig\ln(x/x_0)}-1\right]\frac{d\psi^*}{dx} - \frac{1}{\sqrt{x}}\left[\left(\frac{1}{2}+ig\right)e^{2ig\ln(x/x_0)} - \left(\frac{1}{2}-ig\right)\right]\psi^* \to 0 \tag{73}$$

(as $x \to 0$), where

$$x_0 \equiv \frac{1}{\beta}\left(\frac{G}{J}\right)^{i/2g} \tag{74}$$

is a free constant [38]-the anticipated parameter that characterizes the particular self-adjoint extension. For example, if $\alpha = 0$ (so $g = i/2$), Eq. (73) reduces to

$$\frac{1}{\sqrt{x}}\left[x_0\frac{d\psi}{dx} + \psi\right] \to 0 \tag{75}$$

which is the self-adjoint extension for the free particle on $0 \leqslant x < \infty$. [39]
In the critical case $g = 0(\alpha = 1/4)$ Eq. (65) is replaced by

$$H_0^{(1)}(i\kappa_\pm x) \approx 1 - \frac{\ell_\pm}{2} + \frac{2i}{\pi}\ln(\gamma\beta x/2) \tag{76}$$

[see Eq. (40)], and

$$\phi_\pm \approx A_\pm\sqrt{x}\left[\pm\frac{1}{2} + \frac{2i}{\pi}\ln(\gamma\beta x/2)\right], \tag{77}$$

so

$$\Phi \approx \sqrt{x}[G + J\ln(\gamma\beta x/2)] \tag{78}$$

with

$$G \equiv \frac{1}{2}(A_+ - \lambda A_-) \tag{79a}$$

$$J \equiv \frac{2i}{\pi}(A_+ + \lambda A_-) \tag{79b}$$

and

$$\frac{d\Phi}{dx} \approx \frac{1}{2\sqrt{x}}[G + 2J + J\ln(\gamma\beta x/2)] \tag{80}$$

According to Eq. (64), then, a function ψ is in the selfadjoint domain if

$$\sqrt{x}\ln(x/x_0)\frac{d\psi}{dx} - \frac{1}{\sqrt{x}}\left[1+\frac{1}{2}\ln(x/x_0)\right]\psi \to 0 \tag{81}$$

where in this case $x_0 \equiv (2/\gamma\beta)e^{-G/J}$ is the free parameter characterizing the particular self-adjoint extension. [40]

Where does all this leave us? If we want the $1/x^2$ Hamiltonian, Eq. (50), to be self-adjoint, we must tighten up the naive boundary condition $\psi(0) = 0$, Eq. (4), in favor of a selfadjoint extension [Eq. (73) if $\alpha \neq 1/4$ and Eq. (81) for the critical case $\alpha = 1/4$]. [41] The choice of a particular extension (which is to say, a particular value of x_0) is arbitrary, and in this sense there exists an entire one-parameter family of distinct physical theories described by the $1/x^2$ potential. Question: Do they admit reasonable bound state spectra? We know that the normalized eigenstates of H are given by Eq. (18):

$$\psi_\kappa(x) = A\sqrt{x}K_{ig}(\kappa x) = \frac{i\pi}{2}A\sqrt{x}H_{ig}^{(1)}(i\kappa x) \tag{82}$$

where $\kappa \equiv \sqrt{-2mE}/\hbar$. Which (if any) of these reside in the self-adjoint domain of H?

In the critical case $g = 0$, Eq. (40) yields (for small x)

$$\psi_\kappa(x) \approx -A\sqrt{x}\ln(\gamma\kappa x/2) \tag{83}$$

and

$$\frac{d\psi_\kappa}{dx} \approx -A\frac{1}{\sqrt{x}}\left[1+\frac{1}{2}\ln(\gamma\kappa x/2)\right] \tag{84}$$

Inserting these expressions into Eq. (81) yields the condition $A\ln(\gamma\kappa x_0/2) \to 0$. This holds only if $\gamma\kappa x_0/2 = 1$, which is to say, if $\kappa = 2/\gamma x_0$. Evidently there is exactly one bound state for $\alpha = 1/4$, just as we found (by a completely different route) in Sec. III [Eq. (48)]. But we cannot calculate the allowed energy, because it depends on the arbitrary parameter x_0 (just as, in the renormalization method, it depended on the arbitrary cutoff ϵ).

The case $g \neq 0$ is a little more complicated. Equation (28) gives (for small x)

$$\psi_\kappa(x) \approx B\sqrt{x}\sin\theta \tag{85}$$

where $B \equiv -A\sqrt{\pi/g\sinh(\pi g)}$ and

$$\theta(x) \equiv g\ln(\kappa x/2) - \arg\Gamma(1+ig) \tag{86}$$

It follows that

$$\frac{d\psi_\kappa}{dx} \approx B\frac{1}{\sqrt{x}}\left[\frac{1}{2}\sin\theta + g\cos\theta\right] \tag{87}$$

According to Eq. (73), then, ψ_κ is in the self-adjoint domain if

$$g\ln\left(\frac{2}{\kappa x_0}\right) + \arg\Gamma(1+ig) = n\pi \quad (n = 0, \pm1, \pm2, ...) \tag{88}$$

for g real ($\alpha > 1/4$), or $2/\kappa x_0 = 1$ for g imaginary ($\alpha < 1/4$). In the former case we obtain an infinite set of eigenvalues; in the latter case just one.

Conclusion: To make the $1/x^2$ Hamiltonian self-adjoint we are obliged to impose more stringent boundary conditions [Eq. (73) or (81)] than we naively supposed. This imposition necessarily introduces a free parameter x_0 with the dimensions of length, thereby breaking the

scale invariance of the theory. The result is a reasonable spectrum of allowed states, whose energies, however, we are unable to predict, because they depend on the value of the arbitrary parameter. [42]

V. CONCLUSION

The $1/x^2$ potential is clearly problematic. We can fix it (sort of) by renormalization or by self-adjoint extension, but a reasonable person would likely conclude that the problem itself is artificial and unphysical-maybe there is no such thing as a $1/x^2$ potential in nature. Perhaps some potentials are just plain illegal in quantum mechanics. It seems odd, though, that we never encounter such difficulties in classical mechanics.

Well, in the first place there are classical precursors. [43] Moreover, there do exist systems represented (at least, to good approximation) by a $1/x^2$ potential (at any rate by its three-dimensional analog). The best example is the motion of a charged particle in the field of a stationary electric dipole, for instance, an electron in the vicinity of a polar molecule. Here the potential is $-ep\cos\theta/r^2$, and (surprisingly) the radial Schrödinger equation is mathematically identical to Eq. (2). [44] The critical parameter $\alpha = 1/4$ was noted in early studies of this system, [45] which has attracted renewed attention recently. [46] Like it or not, we have to take this problem seriously.

Comments

[1] Of course, $V(x)$ is unbounded as $x \to 0$, but this by itself is not problematic-the same is true of the Coulomb potential and the delta function well. Our study of the $1/x^2$ potential was inspired by (and in the early parts modeled on) S. A. Coon and B. R. Holstein, "Anomalies in quantum mechanics: The $1/r^2$ potential" Am. J. Phys. 70, 513-519 (2002).
[2] Is there any other potential with this defect? In other words, is there another function of position that contains no dimensional constants and has the same units as $1/x^2$? There is-the two-dimensional delta function, $\delta^2(\mathbf{r}) = \delta(x)\delta(y)$. Our story can be told using the two-dimensional delta function, but because the extra dimension makes the details a little more cumbersome and because the $1/x^2$ potential is arguably more realistic, we prefer to consider it as the model. In fact, for states with circular symmetry the two-dimensional delta function is mathematically equivalent to the $1/x^2$ potential with $\alpha = 1/4$ [Eq. (3)]-see Exercise 1 in Ref. 30. For discussion of the two-dimensional delta function see L. R. Mead, and J. Godines, "An analytical example of renormalization in two-dimensional quantum mechanics," Am. J. Phys. 59, 935-937 (1991); R. Jackiw,
"Delta-function potentials in two- and three-dimensional quantum mechanics," in M. A. B. Bég Memorial Volume, edited by A. Ali and P. Hoodbhoy (World Scientific, Singapore, 1991), pp. 25-42.

[3] Notice that if $\psi(x)$ is normalizable, so too is $\psi_\beta(x)$.

[21] Note that this is a correlated limit in which ϵ and g both go to zero in such a way as to hold κ_1 in Eq. (42) fixed. This is not the same as going straight to $g = 0$ and then letting $\epsilon \to 0$ [Eq. (41)], which only reproduces the limiting value $\pi/4$.
[22] This is not the only way to tame the $1/x^2$ potential. Other regularizations have been proposed. See, for example, C. Schwartz, "Almost singular potentials," J. Math. Phys. 17, 863-867 (1976); H. E. Camblong, L. N. Epele, H. Fanchiotti, and C. A. Garca Canal, "Dimensional transmutation and dimensional regularization in quantum mechanics, I. General theory," and "II. Rotational invariance," Ann. Phys. 287, 14-100 (2001). Our approach follows Ref. 4. It is important in principle to demonstrate that all regularizations lead to the

same physical predictions. If they do not, the theory is non-renormalizable and there is very little that can be done with it.

[23] Of course, if we could detect several bound states, or measure the phase shifts at sufficiently high energy, then we could map out any departures from the $1/x^2$ potential. The question is whether we can make any sense out of the pure $1/x^2$ potential; renormalization offers a means for doing so. By the way, something very similar happens in quantum electrodynamics, where the theory, naively construed, yields an infinite mass for the electron. The introduction of a cutoff renders the mass finite but indeterminate. We take the observed mass of the electron as input and use it to eliminate any explicit reference to the cutoff. The resulting renormalized theory has been spectacularly successful, yielding by far the most precise (and precisely confirmed) predictions in all of physics.
[24] The classic example of an anomaly is the decay of the neutral pion, $\pi^0{}_{25} \to \gamma + \gamma$, which could not occur without the breaking of chiral symmetry.
[25] See, for instance, E. Zeidler, Applied Functional Analysis: Applications to Mathematical Physics (Springer, New York, 1997), pp. 116-117.
[26] Note the logical structure here: We choose $\mathcal{D}_A$, but $\mathcal{D}_{A^\dagger}$ is then determined-it is the space of functions ϕ (in L_2) such that if ψ is in $\mathcal{D}_A$ then Eq. (52) holds.

[32] We assume here that $\alpha < 1/4$; for $\alpha > 1/4$ we could run the same argument using $\psi = \phi = u_+$to obtain the same result.

[33] More explicitly, functions in $\mathcal{D}_H$ vanish if $0 \leqslant x \leqslant \epsilon$ or $x \geqslant \tau$ for arbitrarily small ϵ and arbitrarily large τ.

[34] We follow the treatment in Ref. 30, where the special case $\alpha = 1/4$ is posed as an exercise.

[35] Of course, the eigenvalues of a Hermitian operator are real, so $\phi_+$and ϕ_- cannot be in $\mathcal{D}_H$; rather, the eigenfunctions we seek lie in $\mathcal{D}_{H^+}$.

[36] Mathematicians usually take $\eta = 1$, but this choice offends the physicist's concern for dimensional consistency. In any case, it combines with other arbitrary constants at the end.

[37] This approximation assumes $\mathrm{Re}(ig) > -1/2$, which is fine as long as $\alpha > 0$ (the potential is attractive). It is of some interest to explore selfadjoint extensions of the repulsive $1/x^2$ potential, but we shall not do so here.

[38] Here x_0 is simply a convenient packaging of the arbitrary constants $m, A_\pm$, λ, and η. It is clear from Eq. (73) [if not from Eq. (74)] that x_0 carries the dimensions of length, and hence the choice of a particular self-adjoint extension entails breaking the scale invariance that led to all the difficulties in Sec. II.

[39] This case violates our assumption in Ref. 37, so it should be taken with a grain of salt. See Ref. 30, Example 1, for a more rigorous analysis.

[40] This result agrees with Eq. (80) of Ref. 30, with $r \to x$ and $\varphi \to \psi/x$.

[41] The term "self-adjoint extension" is potentially misleading, because at first sight it appears to involve a contraction, not an expansion, of the domain. The point is that you must

start out with a Hermitian operator, and H is not Hermitian with respect to the set of functions that satisfy the boundary condition $\psi(0) = 0$. That is why we first had to restrict the domain (see Ref. 33), and the "extension" is with respect to that much more limited domain.

[42] By changing the boundary conditions it could be argued that we are radically altering the physical system, albeit at a single point. The process is analogous (in some cases identical) to adding a delta function to the potential, and it is hardly surprising that this changes the spectrum of allowed states. But the question was whether there is anything we could do to salvage the $1/x^2$ potential, and if the remedy is necessarily radical, so be it.

8.5.9 How a Mirror Works from QM Point of View?

(???? как работает зеркало??? пока не знаю, и не время отвечать на этот вопрос.)

8.5.10 Scattering for Systems Described by the Density Matrix

(?? пока не знаю, как это сделать, но мб у Вергелеса в КТП это сделано уже)

8.5.11 Useful Integrals in Scattering Theory and Their Convergence

Примеры вычисления интегралов в теории рассеяния

(очень полезный раздел, а то куча с этим проблем)

9 Typical Addition of Angular Momenta

Обсудим подробно сложение моментов.

9.0.1 Addition of Two Momenta

Суть

Коэффициенты Клебша-Гордана для простейших моментов находятся в таблице от PDG

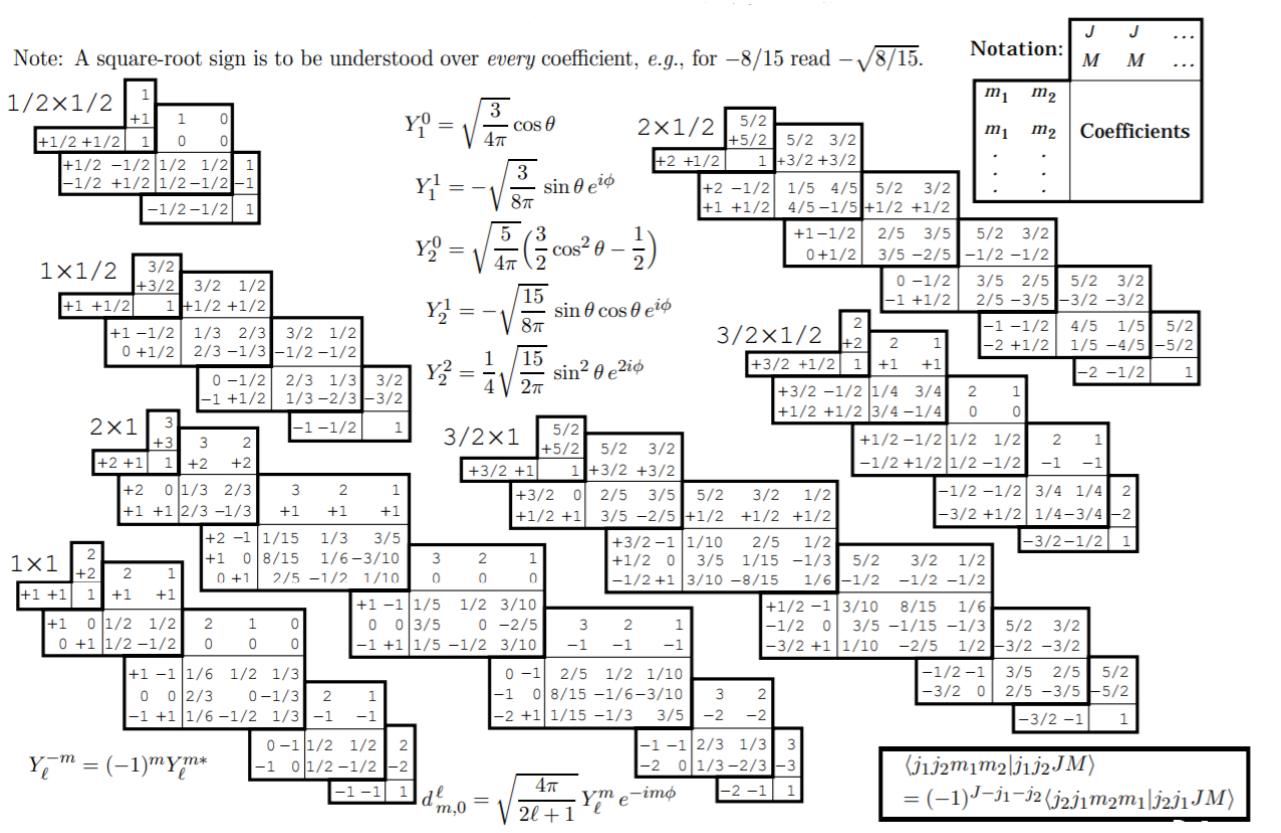


Figure 9.1: PDG таблица коэффициентов Клебша-Гордана

Структура спектра операторов квадрата суммарного момента и проекции момента на выделенную ось

Пусть у нас есть система двух невзаимодействующих моментов l_1 и l_2. Будем считать, что $l_1 \geq l_2$. Найдем суммарный момент такой системы. Каждый из моментов описывается операторами квадрата момента $\hat{L}^2$ и проекции момента на выделенную ось $\hat{L}_z$. Поскольку моменты для каждой системы фиксированы, мы можем работать с этими операторами, суженными на собственные подпространства $\mathbb{C}^{2l_1+1}$ и $\mathbb{C}^{2l_2+1}$ соответственно. Таким образом, мы будем работать с ограниченными операторами. Обозначим эти операторы как $\hat{L}_1^2, \hat{L}_{1,z}, \hat{L}_2^2$ и $\hat{L}_{2,z}$. Напомним, что в базисе из общих собственных векторов операторов $\hat{L}^2$ и $\hat{L}_z$ операторы $\hat{L}_i^2$ и $\hat{L}_{i,z}, i = 1, 2$, - это матрицы с соответствующими собственными числами на главной диагонали. Базисные векторы этих пространств будем обозначать $\psi_m, m = -l_1 ... l_1$, и $\varphi_n, n = -l_2 ... l_2$, то есть нумеровать соответствующим значением проекции момента на выделенную ось.

Подчеркнем здесь, что мы не "ищем" суммарный момент. Наша задача состоит в том, чтобы построить четыре оператора суммарного момента $\hat{L}_\Sigma^2, \hat{L}_{\Sigma,z}, \hat{L}_{\Sigma,x}$ и $\hat{L}_{\Sigma,y}$, обладающих свойствами операторов момента: должны выполняться коммутационные соотношения, и структура спектра должна быть такой же, как у оператора одного момента.

Мы будем строить полный набор наблюдаемых для нашей задачи - операторы квадрата суммарного момента $\hat{L}_\Sigma^2$ и проекции момента на выделенную ось $\hat{L}_{z,\Sigma}$. Поскольку суммарный момент должен обладать всеми свойствами момента, то естественно строить эти операторы как сужение операторов $\hat{L}^2$ и $\hat{L}_z$ на некое подпространство E. Так как моменты не взаимодействуют, то подпространство E совпадает с тензорным произведением $\mathbb{C}^{2l_1+1} \otimes \mathbb{C}^{2l_2+1}$. Размерность пространства E равна $(2l_1 + 1)(2l_2 + 1)$. Базисом в E будет являться множество вида $\{\psi_m \otimes \varphi_n\}$

В пространстве E нам надо выбрать базисные векторы, которые будут общими собственными векторами операторов $\hat{L}_\Sigma^2$ и 14 $\hat{L}_{\Sigma,z}$ (и линейными комбинациями векторов $\{\psi_m \otimes \varphi_n\}$), и присвоить им (из физических соображений) значения собственных чисел этих операторов. Зададим оператор $\hat{L}_{\Sigma,z}$. Мы можем определить

$$\hat{l}_{\Sigma,z} = \hat{L}_{1,z} \otimes \hat{E} + \hat{E} \otimes \hat{L}_{2,z}$$

По аналогии со случаем одного момента введем в пространстве E операторы повышения и понижения проекции суммарного момента на единицу:

$$\hat{L}_- = \hat{L}_{1,-} \otimes \hat{E} + \hat{E} \otimes \hat{L}_{2,-}, \quad \hat{L}_+ = \hat{L}_{1,+} \otimes \hat{E} + \hat{E} \otimes \hat{L}_{2,+},$$

где оператор $\hat{L}_{1,-}$ является оператором понижения проекции первого момента (остальные - соответственно), а оператор $\hat{E}$ - единичный. Отметим, что векторы вида $\psi_{m_1} \otimes \varphi_{m_2}$ являются собственными для оператора $\hat{l}_{\Sigma,z}$ с собственными числами $m_1 + m_2$ соответственно. Каждое их этих собственных чисел, за исключением $\pm(l_1 + l_2)$, вырождено. Назовем максимальной проекцией суммарного момента на ось (то есть первым собственным числом оператора $\hat{L}_{\Sigma,z}$) число $l_1 + l_2$. Соответствующим ему собственным вектором выберем $\psi_{l_1} \otimes \varphi_{l_2}$, который будем обозначать α_1. Легко проверить, что $\hat{L}_+\alpha_1 = 0$. Тогда собственное число оператора $\hat{L}_\Sigma^2$, соответствующее этому собственному вектору, выберем равным $(l_1 + l_2)(l_1 + l_2 + 1)$ Подействовав оператором $\hat{L}_-$на вектор α_1, получим

$$\begin{aligned}\hat{L}_-\alpha_1 = \sqrt{l_1(l_1+1) - l_1(l_1-1)}\psi_{l_1-1} \otimes \varphi_{l_2} + \\ + \sqrt{l_2(l_2+1) - l_2(l_2-1)}\psi_{l_1} \otimes \varphi_{l_2-1}.\end{aligned}$$

Этот вектор после нормировки назовем α_2. Назовем его общим собственным вектором операторов $\hat{L}_\Sigma^2$ и $\hat{L}_{\Sigma,z}$ с собственными значениями $(l_1 + l_2)(l_1 + l_2 + 1)$ и $l_1 + l_2 - 1$ соответственно. Линейная оболочка векторов $\psi_{l_1-1} \otimes \varphi_{l_2}$ и $\psi_{l_1} \otimes \varphi_{l_2-1}$ является двумерным пространством, в котором лежит α_2. Поэтому в нем можно выбрать вектор β_1, ортогональный α_2. Так как сумма магнитных квантовых чисел у базисных векторов β_1 также равна $l_1 + l_2 - 1$, то естественно присвоить этому вектору то же самое значение проекции суммарного момента: $l_1 + l_2 - 1$. Так как на каждом 15 собственном для $\hat{L}^2$ подпространстве оператор $\hat{L}_z$ имеет невырожденный спектр, то суммарное орбитальное квантовое число выберем равным $l_1 + l_2 - 1$, то есть собственное значение оператора $\hat{L}_\Sigma^2$ на этом векторе равно $(l_1 + l_2 - 1)(l_1 + l_2)$. Рассмотрим k-ю степень оператора $\hat{L}_-$:

$$\left(\hat{L}_-\right)^k = \sum_{n=0}^{k} C_k^n \left(\hat{L}_{-,1} \otimes \hat{E}\right)^{k-n} \left(\hat{E} \otimes \hat{L}_{-,2}\right)^n$$

В зависимости от значения k возникают два случая. 1. При $k \leq 2l_2$, действуя оператором понижения 12 на вектор α_1, мы получим линейную комбинацию $k + 1$ попарно ортогональных векторов $\psi_i \otimes \varphi_j, i + j = l_1 + l_2 - k$. Вектору $\left(\hat{L}_-\right)^k \alpha_1$ после нормировки мы присваиваем собственные числа для проекции и квадрата суммарного момента $l_1 + l_2 - k$ и $(l_1 + l_2)(l_1 + l_2 + 1)$ соответственно. Остальным k векторам в этом $k + 1$-мерном подпространстве, ортогональным $\left(\hat{L}_-\right)^k \alpha_1$, присвоим то же значение для проекции момента, а для квадрата момента выберем значения $(l_1 + l_2 - n)(l_1 + l_2 - n + 1), n = \overline{1,k}$. 2. При $2l_2 < k \leq l_1 + l_2$ размерность подпространства, которому принадлежит вектор $\left(\hat{L}_-\right)^k \alpha_1$, остается равной $2l_2 + 1$. Это связано с тем, что вектор

$$\left(\hat{L}_-\right)^{2l_2} \alpha_1$$

имеет в качестве слагаемого элемент $\psi_{l_1} \otimes \varphi_{-l_2}$. Последующее действие на 13 оператора $\hat{L}_-$имеет нулевое слагаемое, так как $\hat{L}_{-,2}\varphi_{-l_2} = 0$. Следовательно, начиная с $k = 2l_2$, оператор 12, действуя на α_1, дает вектор, лежащий в подпространстве одной и той же размерности. Наглядно размерность соответствующего подпространства представлена, например, в [2]. Вектору $\left(\hat{L}_-\right)^k \alpha_1$ мы приписываем собственные числа $l_1 + l_2 - k$ и $(l_1 + l_2)(l_1 + l_2 + 1)$, а $2l_2$ ортогональным им векторам присвоим то же значение для проекции момента, а для квадрата момента выберем значения $(l_1 + l_2 - n)(l_1 + l_2 - n + 1), n = \overline{1, 2l_2}$. Мы видим, что, начиная с $k = 2l_2$, при уменьшении проекции суммарного момента не нужно вводить новых (меньших $l_1 - l_2$) значений для орбитального квантового числа l. Таким образом, мы получили, что минимальное $l = l_1 - l_2$, а минимальное собственное значение оператора $\hat{L}^2_\Sigma$ равно $(l_1 - l_2)(l_1 - l_2 + 1)$ соответственно. Всю эту процедуру можно провести и для оператора повышения проекции момента, стартуя с вектора $\psi_{-l_1} \otimes \varphi_{-l_2}$ с минимальной суммарной проекцией $-(l_1 + l_2)$.

Итак, мы определили спектр операторов квадрата $\hat{L}^2_\Sigma$ и проекции $\hat{L}_{z,\Sigma}$ суммы моментов. Для двух моментов, характеризуемых орбитальными квантовыми числами l_1 и l_2, получено, что суммарный момент характеризуется орбитальными квантовыми числами l, принимающими значения от $l_1 - l_2$ до $l_1 + l_2$. Для каждого такого числа l собственные значения оператора $\hat{L}^2_\Sigma$ равны $l(l+1)$ и $2l+1$ раз вырождены. Собственные числа оператора $\hat{L}_{z,\Sigma}$ при этом принимают значения от $-l$ до l. Суммарная кратность вырождения

$$K = \sum_{n=l_1-l_2}^{l_1+l_2} (2n+1) = (2l_1+1)(2l_2+1)$$

совпадает с размерностью пространства E.

2.2. Построение общего базиса для операторов квадрата суммарного момента и его проекции на выделенную ось

Пока построенный нами базис определен неоднозначно: в каждом подпространстве, соответствующем определенному значению проекции суммарного момента, векторы ортогональны, но иначе никак не фиксированы. Эти векторы определяются однозначно, если потребовать выполнения всех коммутационных соотношений, выполняющихся для одного момента, а именно:

$$\left[\hat{L}^2_\Sigma, \hat{L}_{\Sigma,z}\right] = 0,$$
$$\left[\hat{L}_{\Sigma,x}, \hat{L}_{\Sigma,x}\right] = -i\hat{L}_{\Sigma,y},$$
$$\left[\hat{L}_{\Sigma,y}, \hat{L}_{\Sigma,z}\right] = i\hat{L}_{\Sigma,x},$$
$$\left[\hat{L}^2_\Sigma, \hat{L}_{\Sigma,j}\right] = 0 \quad j = x, y.$$

Причем должно выполняться $\hat{L}_\pm = \hat{L}_{\Sigma,x} \pm i\hat{L}_{\Sigma,y}$. Коммутационное соотношение (14) выполнено автоматически, а вместо соотношений (15) - 17 удобнее рассматривать эквивалентные им

$$\left[\hat{L}^2_\Sigma, \hat{L}_\pm\right] = 0,$$
$$\left[\hat{L}_+, \hat{L}_-\right] = 2\hat{L}_{\Sigma,z},$$
$$\left[\hat{L}_{\Sigma,z}, \hat{L}_\pm\right] = \pm\hat{L}_\pm.$$

Упражнение. Зная, как записываются операторы $\hat{L}_{\pm}$через тензорные произведения операторов $\hat{L}_{\pm,j}, j = 1,2$, а также пользуясь коммутационными соотношениями для последних, доказать соотношения (19) и (20).

Для выполнения (18) необходимо, чтобы действие операторов повышения и понижения не выводили вектор из собственного для конструируемого оператора $\hat{L}^2_\Sigma$ подпространства с фиксированным значением орбитального квантового числа суммарного момента l. Чтобы это гарантировать, будем строить базис из собственных векторов следующим образом. Для собственного подпространства с $l = l_1 + l_2$ собственный вектор с проекцией момента $l_1 + l_2 - n$ равен $\alpha_{n+1} = \left(\hat{L}_-\right)^n \alpha_1, \quad n \leq 2l_1 + 2l_2$, а C выбирается из условия нормировки. Вектор β_1 с $l = l_1 + l_2 - 1$ и максимальной проекцией момента получаем как ортогональный к α_2, а векторы β_n с проекциями $l_1 + l_2 - 1 - n$ для этого l получаем снова как $\beta_{n+1} = \left(\hat{L}_-\right)^n \beta_1, \quad n \leq 2\left(l_1 + l_2 - 1\right)$. И так далее. Если полученные таким образом векторы будут попарно ортогональны друг другу (т.е. образовывать базис), то коммутационное соотношение (18), очевидно, будет выполнено. Докажем ортогональность векторов, соответствующих одной и той же суммарной проекции момента m, но различным орбитальным числам l (ортогональность остальных пар очевидна). То есть докажем, что если $(\alpha_k, \beta_{k-1}) = 0$, то $\left(\hat{L}_-\alpha_k, \hat{L}_-\beta_{k-1}\right) = 0 \quad \forall k = \overline{2, 2l-1}$:

$$\left(\hat{L}_-\alpha_k, \hat{L}_-\beta_{k-1}\right) = \left(\alpha_k, \hat{L}_+\hat{L}_-\beta_{k-1}\right) = \left(\alpha_k, \hat{L}_+\beta_k\right) = \\ = (\alpha_k, \text{ const } \cdot \beta_{k-1}) = 0.$$

Мы показали, что векторы, соответствующие одной и той же проекции момента, ортогональны. Тем самым доказана верность коммутационного соотношения 18, что и завершает построение оператора суммарного момента. Построенные векторы образуют ортонормированный базис, каждый вектор которого мы можем индексировать соответствующими значениями орбитального и магнитного квантовых чисел суммарного момента $\Psi_{l_\Sigma, m_\Sigma}$. Определенные на этом базисе операторы $\hat{L}_{\Sigma,i}, i = 1,2,3$, и $\hat{L}^2_\Sigma$ имеют структуру спектра операторв момента и удовлетворяют коммутационным соотношениям 17.

Если обозначить как $\mathbb{J}_k$ собственное подпространство операторов $\hat{L}^2$ и $\hat{L}_z$ со значением орбитального квантового числа $l = k$, то удобно работать не с пространством $\mathbb{C}^{2l_1+1} \otimes \mathbb{C}^{2l_2+1}$, а с изометрически изоморфным ему

Определив для каждого значения $k \in [(l_1 - l_2), ..., (l_1 + l_2)]$ диагональные матрицы размера $(2k+1) \times (2k+1)$:

$$B_k = \begin{pmatrix} k & & \\ & \ddots & \\ & & -k \end{pmatrix}, \quad D_k = \begin{pmatrix} k(k+1) & & \\ & \ddots & \\ & & k(k+1) \end{pmatrix}$$

получим в пространстве (21) блочно-диагональные матрицы опе- 19 ратора проекции суммарного момента

$$\begin{pmatrix} B_{l_1+l_2} & & \\ & \ddots & \\ & & B_{l_1-l_2} \end{pmatrix}$$

и оператора квадрата суммарного момента

$$\begin{pmatrix} D_{l_1+l_2} & & \\ & \ddots & \\ & & D_{l_1-l_2} \end{pmatrix}.$$

Пример 11. Суммарный момент электрона со спином $1/2$ и орбитальным моментом $l = 1$.

Нужно просуммировать моменты $l = 1$ и $s = 1/2$. Пространство $E = \mathbb{C}^{2\cdot 1+1} \otimes \mathbb{C}^{2\cdot 1/2+1}$, размерность равна 6. Базис в пространстве состоит из векторов

$$\psi_1 \otimes \varphi_{1/2} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \psi_1 \otimes \varphi_{-1/2} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\psi_0 \otimes \varphi_{1/2} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \psi_0 \otimes \varphi_{-1/2} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\psi_{-1} \otimes \varphi_{1/2} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \psi_{-1} \otimes \varphi_{-1/2} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Структура спектра ясна из приведенных выше общих рассуждений: орбитальное число l_Σ суммарного момента должно принимать значения $1/2$ (что соответствует $l - s$) и $3/2$ (что соответствует $l + s$). Других значений нет, так как $l - s + 1$ совпадает с максимальным значением суммарного момента. Соответствующие собственные числа оператора $\hat{L}^2_\Sigma$ равны $(l + s)(l + s + 1) = 15/4$ с кратностью вырождения $2(l + s) + 1 = 4$ и $(l - s)(l - s + 1) = 3/4$ с кратностью вырождения $2(l - s) + 1 = 2$. Таким образом, собственные числа оператора $\hat{L}^2_\Sigma$ равны

$$\left\{\frac{15}{4}, \frac{15}{4}, \frac{15}{4}, \frac{15}{4}, \frac{3}{4}, \frac{3}{4}\right\},$$

20 а собственные числа $\hat{L}_{\Sigma,z}$ равны

$$\left\{\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}\right\}.$$

Построим собственные векторы:

$$\alpha_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \Psi_{3/2,3/2}$$

Действуем оператором понижения $\hat{L}_- = \hat{L}_{-,1} \otimes \hat{E} + \hat{E} \otimes \hat{s}_-$на вектор α_1:

$$\hat{L}_-\alpha_1 = \sqrt{2}\psi_0 \otimes \varphi_{1/2} + \psi_1 \otimes \varphi_{-1/2}$$

Нормируем этот вектор:

$$\begin{aligned}
&\left\|\sqrt{2}\psi_0 \otimes \varphi_{1/2} + \psi_1 \otimes \varphi_{-1/2}\right\|^2 = \\
&= \left(\sqrt{2}\psi_0 \otimes \varphi_{1/2} + \psi_1 \otimes \varphi_{-1/2}, \sqrt{2}\psi_0 \otimes \varphi_{1/2} + \psi_1 \otimes \varphi_{-1/2}\right) = \\
&= \left(\sqrt{2}\psi_0 \otimes \varphi_{1/2}, \sqrt{2}\psi_0 \otimes \varphi_{1/2}\right) + \left(\sqrt{2}\psi_0 \otimes \varphi_{1/2}, \psi_1 \otimes \varphi_{-1/2}\right) + \\
&\quad + \left(\psi_1 \otimes \varphi_{-1/2}, \sqrt{2}\psi_0 \otimes \varphi_{1/2}\right) + \left(\psi_1 \otimes \varphi_{-1/2}, \psi_1 \otimes \varphi_{-1/2}\right) = \\
&= 2\left(\psi_0, \psi_0\right)\left(\varphi_{1/2}, \varphi_{1/2}\right) + \left(\psi_1, \psi_1\right)\left(\varphi_{-1/2}, \varphi_{-1/2}\right) = 3
\end{aligned}$$

Тогда

$$\alpha_2 = \sqrt{\frac{2}{3}}\psi_0 \otimes \varphi_{1/2} + \sqrt{\frac{1}{3}}\psi_1 \otimes \varphi_{-1/2}.$$

Этот вектор соответствует собственным числам 15/4 и 1/2 (орбитальное квантовое число 3/2), и его можно обозначить $\Psi_{3/2,1/2}$. Ортогональный ему вектор в подпространстве $\mathrm{Lin}\left\{\psi_0 \otimes \varphi_{1/2}, \psi_1 \otimes \varphi_{-1/2}\right\}$ также будет иметь проекцию 1/2, но орбитальное квантовое число 1/2, поэтому сразу назовем его $\alpha_5 = c_1 \cdot \psi_0 \otimes \varphi_{1/2} + c_2 \cdot \psi_1 \otimes \varphi_{-1/2}$. Постоянные определяются условиями $(\alpha_2, \alpha_5) = 0$ и $\|\alpha_5\| = 1 : c_1 = \frac{1}{\sqrt{3}}, c_2 = -\sqrt{\frac{2}{3}}$. Нормированный α_5 обозначим $\Psi_{1/2,1/2}$. Орбитальному квантовому числу 3/2 и минимальной проекции момента $-3/2$ соответствует только один вектор: $\alpha_4 = \psi_{-1} \otimes \varphi_{-1/2} = \Psi_{3/2,-3/2}$. Действуя на него оператором повышения, получим

$$\hat{L}_+\alpha_4 = \sqrt{2}\psi_0 \otimes \varphi_{-1/2} + \psi_{-1} \otimes \varphi_{1/2}$$

и тогда

$$\alpha_3 = \sqrt{\frac{2}{3}}\psi_0 \otimes \varphi_{-1/2} + \sqrt{\frac{1}{3}}\psi_{-1} \otimes \varphi_{1/2} = \Psi_{3/2,-1/2}.$$

Последний нормированный вектор α_6 из соображений ортогональности α_3 в подпространстве $\mathrm{Lin}\left\{\psi_0 \otimes \varphi_{-1/2}, \psi_{-1} \otimes \varphi_{1/2}\right\}$ paBeH

$$\alpha_6 = \frac{1}{\sqrt{3}}\psi_0 \otimes \varphi_{-1/2} - \sqrt{\frac{2}{3}}\psi_{-1} \otimes \varphi_{1/2} = \Psi_{1/2,-1/2}$$

Базисные векторы $\{\Psi_{l_\Sigma,m_\Sigma}\}$ вместе с собственными значениями (22) и 23 задают операторы $\hat{L}^2_\Sigma$ и $\hat{L}_{\Sigma,z}$ на пространстве $\mathbb{C}^3 \otimes \mathbb{C}^2$. Матрицы $\hat{L}_{\Sigma,x}$ и $\hat{L}_{\Sigma,y}$ можно записать с помощью операторов $\hat{L}_\pm$, записанных в построенном базисе. Как было доказано в пункте 2.1, построенные таким образом операторы будут удовлетворять коммутационным соотношениям для операторов одного момента. Построим естественный изоморфизм $U : \mathbb{C}^3 \otimes \mathbb{C}^2 \to \mathbb{J}_{3/2} \oplus \mathbb{J}_{1/2}$:

$$U\left(\psi_1 \otimes \varphi_{1/2}\right) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$U\left(\sqrt{\frac{2}{3}}\psi_0 \otimes \varphi_{1/2} + \sqrt{\frac{1}{3}}\psi_1 \otimes \varphi_{-1/2}\right) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

и так далее. Тогда операторы суммарного момента в этом базисе запишутся как

$$\hat{L}_{\Sigma,z} = \begin{pmatrix} 3/2 & & & & & \\ & 1/2 & & & & \\ & & -1/2 & & & \\ & & & -3/2 & & \\ & & & & 1/2 & \\ & & & & & -1/2 \end{pmatrix}.$$

У пражнение. Постройте операторы суммарного спина для двух частиц со спином 1/2. Докажите, что $\hat{S}_\Sigma$ не коммутирует с $\hat{S}_{1,z}$. Покажите, что эти операторы коммутируют на каждом собственном для $\hat{S}_\Sigma$ подпространстве. 2.3. Восстановление волновых функций в координатном представлении

В результате процедуры сложения двух моментов мы получили векторы $\Psi_{L,M}$. Интересно восстановить этот вектор в координатном представлении, так как именно в нем мы получим плотности распределения того или иного состояния по координате.

Пример 12. Суммарный момент двух невзаимодействующих частиц, каждая их которых находится в состоянии с моментом, имеющим орбитальное квантовое число 1. Базис состояний для каждой частицы - это векторы $\psi_{1,m}$ и $\varphi_{1,m}$, где $m = \{-1, 0, 1\}$. В координатном представлении базис состояний записывается как $\{Y_1^{m_1}(\theta_1, \varphi_1)\}$ и $\{Y_1^{m_2}(\theta_2, \varphi_2)\}$, где $m = \{-1, 0, 1\}$, а $Y_l^m(\theta, \varphi)$ - сферические функции.

Общий вектор суммарного момента, соответствующий, например, пример, квантовым числам $L = 2$ и $M = 1$, равен

$$\Psi_{2,1} = \frac{\psi_{1,0} \otimes \varphi_{1,1} + \psi_{1,1} \otimes \varphi_{1,0}}{\sqrt{2}}$$

В координатном представлении этот вектор запишется как

$$\Psi_{2,1}(\theta_1, \varphi_1, \theta_2, \varphi_2) =$$
$$= \frac{1}{\sqrt{2}} \left(Y_1^0(\theta_1, \varphi_1) Y_1^1(\theta_2, \varphi_2) + Y_1^1(\theta_1, \varphi_1) Y_1^0(\theta_2, \varphi_2) \right).$$

Пример 13. Суммарный момент частицы с моментом 1 и спином 1/2.

Воспользуемся результатами Примера 11. Запишем, например, вектор $\Psi_{3/2,1/2}$ в координатном представлении. Векторы, описывающие состояние проекции спина, не могут быть записаны в координатном представлении, так как они конструируются сразу в собственном представлении (отражение чисто квантовой природы спина), то интересующий нас вектор записывается в виде разложения волновой функции по собственным векторам проекции спина на ось OZ:

$$\Psi_{3/2,1/2}(\theta, \varphi) = \begin{pmatrix} \sqrt{\frac{2}{3}} Y_1^0(\theta, \varphi) \\ \sqrt{\frac{1}{3}} Y_1^1(\theta, \varphi) \end{pmatrix}.$$

§3. Соотношения ортогональности для коэффициентов Клебша-Гордана

Определение 14. Коэффициенты $K^{l_\Sigma, m_\Sigma}_{l_1, m_1, l_2, m_2}$ разложения базиса $\Psi_{l_\Sigma, m_\Sigma}$ по базису $\{\psi_{m_1} \otimes \varphi_{m_2}\}$ называются коэффициентами Клебша-Гордана.

Нередко индексы l_1 и l_2 опускаются для каждой определенной задачи, в которой они фиксированы.

Пример 15. Коэффициенты Клебша-Гордана для Примера 11 обозначим $K^{l_\Sigma, m_\Sigma}_{m, s_m}$, где число m - проекция на выделенную ось момента l, s_m - проекция на ту же ось спина электрона, l_Σ - орбитальное квантовое число суммарного момента, m_Σ - проекция су|ммарного момента. Первая пара аргументов характеризует старый базис $\psi_i \otimes \varphi_j$, а вторая пара аргументов - новый базис α_k. Выше мы нашли, что

$$K^{3/2,3/2}_{1,1/2} = 1, \quad K^{3/2,1/2}_{0,1/2} = \sqrt{\frac{2}{3}}, \quad K^{3/2,1/2}_{1,-1/2} = \frac{1}{\sqrt{3}}, \quad \text{etc.}$$

Утверждение 16. Коэффициенты Клебша-Гордана удовлетворяют "условию ортогональности":

$$\sum_{m_1,m_2} K^{L,M}_{m_1,m_2} K^{L',M'}_{m_1,m_2} = \delta_{LL'}\delta_{MM'}$$

Доказательство. Векторы Ψ_{LM} и $\Psi_{L'M'}$ ортогональны, если не совпадает хотя бы одна пара индексов:

$$\delta_{LL'}\delta_{MM'} = (\Psi_{LM}, \Psi_{L'M'}) =$$

$$= \left(\sum_{m_1,m_2} K^{LM}_{m_1,m_2} \psi_{m_1} \otimes \varphi_{m_2}, \sum_{m'_1,m'_2} K^{L'M'}_{m'_1,m'_2} \psi_{m'_1} \otimes \varphi_{m'_2} \right) =$$

$$= \sum_{m_1,m_2} \sum_{m'_1,m'_2} K^{LM}_{m_1,m_2}, K^{L'M'}_{m'_1,m'_2} \left(\psi_{m_1} \otimes \varphi_{m_2}, \psi_{m'_1} \otimes \varphi_{m'_2} \right) =$$

$$= \sum_{m_1,m_2} K^{LM}_{m_1,m_2} K^{L'M'}_{m_1,m_2}$$

что и доказывает утверждение.

Утверждение 17. Коэффициенты Клебша-Гордана удовлетворяют "условию ортогональности":

$$\sum_{L,M} K^{L,M}_{m_1,m_2} K^{L,M}_{m'_1,m'_2} = \delta_{m_1 m'_1}\delta_{m_2 m'_2}$$

Доказательство. Матрица, составленная из коэффициентов Клебша-Гордана $K^{LM}_{m_1 m_2}$, осуществляет изометрический изоморфизм пространства $\mathbb{C}^{2l_1+1} \otimes \mathbb{C}^{2l_2+1}$ на пространство $\bigoplus_{k=l_1-l_2}^{l_1+l_2} \mathbb{J}_k$. Компоненты матрицы обратного преобразования обозначим $\tilde{K}^{m_1 m_2}_{LM}$. Заметим, что

$$\tilde{K}^{m_1 m_2}_{LM} = (\Psi_{LM}, \psi_{m_1} \otimes \varphi_{m_2}) = K^{LM}_{m_1 m_2}$$

Доказательство утверждения следует из равенства

$$\delta_{m_1 m'_1}\delta_{m_2 m'_2} = \left(\psi_{m_1} \otimes \varphi_{m_2}, \psi_{m'_1} \otimes \varphi_{m'_2} \right) =$$
$$= \sum_{LM} K^{LM}_{m_1 m_2} K^{LM}_{m'_1 m'_2}$$

9.0.2 Wigner–Eckart Theorem

Теория

Теорема Вигнера-Эккарта является важным техническим инструментом в задачах квантовой механики. Для ее правильного применения необходимо понимать утверждение теоремы. Учебники квантовой механики, такие как [1, 3], предполагают при формулировании теоремы дополнительную подготовку студентов в этом вопросе. В частности, доказательство и применение теоремы Вигнера-Эккарта предполагает как минимум знакомство с теорией групп. Для нужд второго семестра квантовой механики, изучаемой в МФТИ, эта теорема может быть сформулирована и доказана без аппеляции к этому разделу математики. Ниже приводится доказательство этой теоремы по книге |2| и ее применение к вычислению фактора Ланде и получению правил отбора для дипольного излучения. Приведенное доказательство предполагает хорошее знакомство читателя с процедурой построения оператора суммарного момента.

Здесь и далее в основном используются обозначения Дирака. Будем обозначать общий собственный для некоторого полного набора наблюдаемых П вектор какого-либо

гильбертова пространства $\mathcal{H}$ его индексами - квантовыми числами соответствующего полного набора наблюдаемых $-|a_1, a_2, ..., a_n\rangle$. Такое обозначение не конкретизирует пространство $\mathcal{H}$, то есть какое-то определенное представление. В этом случае говорят, что вектор $|a_1, a_2, ..., a_n\rangle$ лежит в "абстрактном гильбертовом пространстве". Мы также будем работать с определенным представлением. В этом случае будем обозначать как $\Psi_{a_1,...,a_n}$ волновую функ- цию в этом представлении. Например, вектор $|1, 0\rangle$, собственный для операторов орбитального момента $\hat{L}^2$ и проекции момента на ось $OZ\hat{L}_z$, заданный орбитальным квантовым числом $l = 1$ и магнитным квантовым числом $m = 0$, в координатном представлении записывается как

$$\Psi_{1,0}(\theta, |\varphi) = \langle\theta, \varphi|1, 0\rangle = \sqrt{\frac{3}{4\pi}}\cos\theta.$$

Этот же вектор $|1, 0\rangle$ в собственном представлении для $l = 1$, $m = \{1, 0, -1\}$, может быь записан в виде

$$\Psi_{1,0} = \langle 1, m|1, 0\rangle = \{0, 1, 0\} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

При этом запись, например, $\left\langle JM'|\hat{A}|JM\right\rangle \in \mathbb{C}$ и означает скалярное произведение $\left(\Psi_{J,M'}, \hat{A}\Psi_{J,M}\right)$.

Ниже мы используем стандартно определенные [1, 3] операторы орбитального момента $\hat{L}^2, \hat{L}_i, i = 1, 2, 3, \hat{L}_\pm$, операторы спина $\hat{S}^2, \hat{S}_i, i = 1, 2, 3, \hat{S}_\pm$, и оперторы суммарного момента $\hat{J}^2, \hat{J}_i,\ i = 1, 2, 3, \hat{J}_\pm$.

Сферические тензоры

Определение 1 сферического тензора. Пусть операторы $\hat{T}^{(k)}_q, q \in [-k, k]$, определены на собственном для $\hat{J}^2$ подпространстве $\mathbb{J}_K$ или на конечной прямой сумме таких подпространств [4]:

$$\bigoplus_{J=K}^{J=N} \mathbb{J}_K$$

Набор операторов $\hat{T}^{(k)}_q, q \in [-k, k]$, будем называть сферическим тензором, если выполнены следующие коммутационные соотношения: 1. $\left[\hat{J}_\pm, \hat{T}^{(k)}_q\right] = C_\pm(k, q)\hat{T}^{(k)}_{q\pm1}$ 2. $\left[\hat{J}_z, \hat{T}^{(k)}_q\right] = q\hat{T}^{(k)}_q$. Замечание 2. Обратите внманиние, что так как мы определили операторы $\hat{T}^{(k)}_q$ на конечномерном подпространстве гильбертова пространства $\mathcal{H}$, то мы работаем с ограниченными операторами, при определении коммутации которых не возникает тех проблем, которые свойственны определению коммутатора неограниченных операторов в бесконечномерном пространстве.

В рассматриваемом нами случае коммутация операторов, определенных на конечномерных подпространствах гильбертова пространства, совпадает с перестановочностью матриц.

Определение 3. Постоянные $C_\pm(k, q) = \sqrt{(k \mp q)(k \pm q + 1)}$ - стандартные коэффициенты при действии операторов повышения/понижения момента $\hat{J}_\pm$на общие для операторов квадрата $\hat{J}^2$ и проекции момента $\hat{J}_z$ собственные векторы $|j, m\rangle$.

Приведем примеры сферических тензоров, которые мы будем использовать в дальнейшем.

Пример 4. Для вычисления фактора Ланде нам понадобятся матричные элементы $\left\langle JM' \left| \hat{1} \otimes \hat{S}_z \right| JM \right\rangle$. Поэтому сделаем предположение, что мы можем ввести сферический тензор $\hat{A}_q^{(k)}$ с $k = 1$ и $\hat{A}_0^{(1)} = \hat{1} \otimes \hat{S}_z$. Найдем остальные компоненты $\hat{A}_{\pm 1}^{(1)}$. По Определению 1] сферического тензора для набора операторов $\hat{A}_q^{(1)}$, $q = -1, 0, 1$, должно быть выполнено

$$\left[\hat{J}_\pm, \hat{A}_0^{(1)}\right] = C_\pm(1,0)\hat{A}_{\pm 1}^{(1)} = \sqrt{2}\hat{A}_{\pm 1}^{(1)}$$

Вычислим, чему равен на самом деле коммутатор в левой части этого равенства:

$$\left[\hat{J}_\pm, \hat{1} \otimes \hat{S}_z\right] = \left[\hat{L}_\pm \otimes \hat{1} + \hat{1} \otimes \hat{S}_\pm, \hat{1} \otimes \hat{S}_z\right] = \mp \hat{1} \otimes \hat{S}_\pm$$

Таким образом,

$$\hat{A}_{\pm 1}^{(1)} = \mp \frac{1}{\sqrt{2}} \hat{1} \otimes \hat{S}_\pm.$$

Упражнение. Пользуясь Определением 3 и выражениями (1), проверьте самостоятельно выполнение остальных 7 коммутационных соотношений в Определении 1:

$$\begin{gathered}
\left[\hat{J}_+, \hat{A}_{+1}^{(1)}\right] = 0, \\
\left[\hat{J}_+, \hat{A}_{-1}^{(1)}\right] = \sqrt{2}\hat{A}_0^{(1)}, \\
\left[\hat{J}_-, \hat{A}_{+1}^{(1)}\right] = \sqrt{2}\hat{A}_0^{(1)}, \\
\left[\hat{J}_-, \hat{A}_{-1}^{(1)}\right] = 0,
\end{gathered}$$

$$\begin{gathered}
\left[\hat{J}_z, \hat{A}_0^{(1)}\right] = 0, \\
\left[\hat{J}_z, \hat{A}_{+1}^{(1)}\right] = \hat{A}_{+1}^{(1)}, \\
\left[\hat{J}_z, \hat{A}_{-1}^{(1)}\right] = \hat{A}_{-1}^{(1)}.
\end{gathered}$$

Пример 5. Для правил отбора для дипольного излучения нам понадобятся матричные элементы компонент дипольного момента $\left\langle JM' \left| \hat{d}_i \right| JM \right\rangle$. Выберем в качестве нулевой компоненты сферического тензора $\hat{B}_0^{(1)} = \hat{d}_z$. Тогда из коммутационных соотношений [2] получим

$$\hat{B}_{\pm 1}^{(1)} = \mp \frac{1}{\sqrt{2}} \left(\hat{d}_x \pm i\hat{d}_y \right) = \mp \frac{1}{\sqrt{2}} \hat{d}_\pm.$$

У пражнение. Проверьте все коммутационные соотношения из Определения 1. Для этого покажите, что все собственные функции операторов проекции момента лежат в области опеределения операторов $\hat{x}_i$. Покажите, что для суженных на собственные для $\hat{L}^2$ подпространства операторов $\hat{x}_i$ выполнены нужные коммутационные соотношения. Покажите, что соотношения из Определения 1 выполнены и для операторов $\hat{J}_i$.

Пример 6. В частности, и сами компоненты оператора момента образуют сферический тензор:

$$\begin{aligned}
\hat{C}_0^{(1)} &= \hat{J}_z, \\
\hat{C}_{\pm 1}^{(1)} &= | \mp \frac{1}{\sqrt{2}} \hat{J}_\pm.
\end{aligned}$$

Теорема Вигнера-Эккарта

Теорема 7 Вигнера-Эккарта.

Пусть $\hat{T}_q^{(k)}, q \in [-k,k]$ для фиксированного k, - сферический тензор. Тогда матричный элемент каждой компоненты сферического тензора $\left\langle j', m' \left| \hat{T}_q^{(k)} \right| j, m \right\rangle$ пропорционален соответствующему коэффициенту Клебша-Гордана $K_{j,m;k,q}^{j',m'}$[1, 3, 4], а коэффициент пропорциональности Λ не зависит от квантовых чисел m, m', q и может зависеть лишь только от j, j', k:

$$\left\langle j', m' \left| \hat{T}_q^{(k)} \right| j, m \right\rangle = \Lambda\left(j, j', k\right) K_{j,m;k,q}^{j',m'}$$

Здесь $K_{j,m;k,q}^{j',m'} = \langle j', m' | j, m; k, q \rangle$ - коэффициенты Клебша-Гордана сложения моментов j и k|4|. Так как эти квантовые числа фиксированы, то в дальнейшем будем их опускать в записи коэффициентов:

$$K_{j,m;k,q}^{j',m'} \equiv K_{mq}^{j'm'}$$

Доказательство. А. Докажем реккурентные соотношения для коэффициентов Клебша-Гордана. При сложении моментов j и k получаем значения квантового числа j', характеризующего суммарный момент: $j' = |j-k|...(j+k)$. Подействуем операторами повышения/понижения суммарного момента $\hat{J}_\pm$на собственный вектор суммарного момента $|j', m'\rangle$:

$$\hat{J}_\pm \left|j', m'\right\rangle = C_\pm\left(j', m'\right) \left|j', (m' \pm 1)\right\rangle$$

С другой стороны, мы, во-первых, можем записать вектор суммарного момента через коэффициенты Клебша-Гордана и собственные векторы складываемых моментов:

$$|j', m'\rangle = \sum_{m_1, m_2} K_{m_1 m_2}^{j'm'} |j, m_1\rangle \otimes |k, m_2\rangle$$

а во-вторых, сам оператор повышения/понижения переписать в виде суммы соответствующих операторов для первого и второго моментов:

$$\hat{J}_\pm = \hat{j}_{1,\pm} \otimes \hat{1} + \hat{1} \otimes \hat{j}_{2,\pm}$$

Тогда получаем равенство

$$\begin{aligned} C_\pm\left(j', m'\right) \left|j', (m' \pm 1)\right\rangle = \\ = \sum_{m_1, m_2} K_{m_1 m_2}^{j'm_2'} \left[C_\pm\left(j, m_1\right) \left|j, (m_1 \pm 1)\right\rangle \otimes |k, m_2\rangle + \right. \\ \left. + C_\pm\left(k, m_2\right) |j, m_1\rangle \otimes \left|k, (m_2 \pm 1)\right\rangle\right]. \end{aligned}$$

Умножим полученное равенство слева на вектор $\langle j, m| \otimes \langle k, q|$:

$$C_\pm\left(j', m'\right) K_{mq}^{j'(m'\pm1)} = C_\pm(j, m \mp 1) K_{(m\mp1)q}^{j'm'} + C_\pm(k, q \mp 1) K_{m(q\mp1)}^{j'm'}.$$

Заметим, что

$$\begin{aligned} C_\pm(j, m \mp 1) = \sqrt{[j \mp (m \mp 1)][j \pm (m \mp 1) + 1]} = \\ = \sqrt{(j \mp m + 1)(j \pm m)} = C_\mp(j, m). \end{aligned}$$

Окончательно получаем реккурентные соотношения для коэффициентов Клебша-Гордана в виде

$$C_\pm\left(j', m'\right) K_{mq}^{j'(m'\pm1)} = C_\mp(j, m) K_{(m\mp1)q}^{j'm'} + C_\mp(k, q) K_{m(q\mp1)}^{j'm'}.$$

B. Получим подобные соотношения для матричных элементов компонент сферического тензора. Для этого рассмотрим матричный элемент коммутатора

$$\left\langle j', m' \left| \left[\hat{J}_{\pm}, \hat{T}_q^{(k)} \right] \right| j, m \right\rangle .$$

С одной стороны, запишем этот матричный элемент, воспользовавшись коммутационным соотношением из определения сферического тензора:

$$\left\langle j', m' \left| \left[\hat{J}_{\pm}, \hat{T}_q^{(k)} \right] \right| j, m \right\rangle = C_{\pm}(k, q) \left\langle j', m' \left| \hat{T}_{q\pm1}^{(k)} \right| j, m \right\rangle .$$

С другой стороны, мы можем воспользоваться непосредственно определением коммутатора и определением операторов, сопря- 10 женных к операторам $\hat{J}_{\pm}$:

$$\begin{gathered} \left\langle j', m' \left| \left[\hat{J}_{\pm}, \hat{T}_q^{(k)} \right] \right| j, m \right\rangle = \\ = C_{\mp}(j', m') \left\langle j', m' \mp 1 \left| \hat{T}_q^{(k)} \right| j, m \right\rangle - \\ - C_{\pm}(j, m) \left\langle j', m' \left| \hat{T}_q^{(k)} \right| j, m \pm 1 \right\rangle . \end{gathered}$$

Заметив, что

$$C_{\mp}(j, m) = C_{\pm}(j, -m),$$

получаем

$$\begin{gathered} C_{\pm}(j', -m') \left\langle j', m' \mp 1 \left| \hat{T}_q^{(k)} \right| j, m \right\rangle = \\ = C_{\mp}(j, -m) \left\langle j', m' \left| \hat{T}_q^{(k)} \right| j, m \pm 1 \right\rangle + \\ + C_{\mp}(k, -q) \left\langle j', m' \left| \hat{T}_{q\pm1}^{(k)} \right| j, m \right\rangle . \end{gathered}$$

Делая в этом выражении замену $m \to -m, m' \to -m'$ и $q \to -q$, приходим к равенству

$$\begin{gathered} C_{\pm}(j', m') \left\langle j', -(m' \pm 1) \left| \hat{T}_{-q}^{(k)} \right| j, -m \right\rangle = \\ = C_{\mp}(j, m) \left\langle j', -m' \left| \hat{T}_{-q}^{(k)} \right| j, -(m \mp 1) \right\rangle + \\ + C_{\mp}(k, q) \left\langle j', -m' \left| \hat{T}_{-(q\mp1)}^{(k)} \right| j, -m \right\rangle . \end{gathered}$$

C. Система (2) - система линейных уравнений на коэффициенты Клебша-Гордана $K_m^{j'm'}$. Эта система была получена действием операторов повышения/понижения на собственные векторы суммарного момента. Так как эти операторы действуют только на собственных для $\hat{J}^2$ подпространствах (переход между подпространствами осуществляется поиском ортогонального вектора, [4]), то эти реккурентные соотношения верны для фиксированных j, j' и k. 11 Система (2) является линейной однородной системой с известными коэффициентами $C_{\pm}(j, m)$ для поиска коэффициентов Клебша-Гордана $K_{mq}^{j'm'}$, которые можно нумеровать сквозным параметром $i = \{m, m', q\} : K_{mq}^{j''} = K_i(j, j', k)$. Найденные коэффициенты Клебша-Гордана будем называть вектором решения, понимая под термином "вектор" не объект с определёнными трансформационными свойствами при замене координат, а просто набор чисел, нумеруемых индексом i.

Из процедуры сложения моментов для каждого фиксированного j' точно известны коэффициенты Клебша-Гордана, если мы нормируем хотя бы один собственный вектор суммарного момента. При решении системы (2) нормировки вектора не происходит, и, значит, коэффициенты Клебша-Гордана находятся с точностью до одного для всех

постоянного множителя. Значит, решение системы (2) образует одномерное пространство.

Система (3) - та же самая линейная система с теми же коэффициентами, но на поиск матричных элементов сферического тензора. Только что было показано, что решение этой системы является одномерным. Значит, матричные элементы должны быть пропорциональны соответствующим коэффициентам Клебша-Гордана. Коэффициент пропорциональности Λ не может зависеть от индекса i, нумерующего компоненту вектора решения, то есть Λ не зависит от m, m' и q, и может зависеть только от внешних параметров системы $-j, j'$ и k. Значит, мы можем записать:

$$\left\langle j', -m' \left| \hat{T}^{(k)}_{-(q\mp1)} \right| j, -m \right\rangle = \Lambda\left(j, j', k\right) K^{j',m'}_{j,m;k,(q\mp1)}.$$

Окончательно, меняя знак у проекции моментов в левой части равенства и обозначая $q' = (q \mp 1)$, получаем стандартную форму утверждения теоремы Вигнера-Эккарта:

$$\left\langle j', m' \left| \hat{T}^{(k)}_{q'} \right| j, m \right\rangle = \Lambda\left(j, j', k\right) K^{j',m'}_{j,m;k,q'}$$

Тем самым теорема доказана.

Матричный элемент неприводимого тензорного оператора $T^{(j)}_m$

что это???

пока что так и не въехал.

теорема Вигнера-Эккарта

теорема Вигнера-Эккарта утверждает, что матричный элемент неприводимого тензорного оператора $T^{(j)}_m$ порядка j с проекцией m по состояниям с заданными значениям и момента выражается через коэффициенты Клебша-Гордона в виде

$$\left\langle J, M \left| T^{(j)}_m \right| J', M' \right\rangle = \frac{\left\langle J \left\| T^{(j)} \right\| J' \right\rangle}{\sqrt{2J+1}} \left\langle J, M | J', M'; j, m \right\rangle$$

где $\left\langle J \left\| T^{(j)} \right\| J' \right\rangle$ -приведенный матричный элемент оператора, который зависит только ОТ J и J', но не зависит от проекций моментов.

Здесь фактор $1/\sqrt{2J+1}$ введен согласно общепринятому соглашению для удобства при вычислениях.

Мы по существу доказали эту теорему явным построением неприводимых тензорных Операторов общего вида [5], затем определив их трансформационные свойства.

Обычно поступают наоборот, постулируют закон преобразования величин при вращениях и отсюда получают общий вид оператора, т.е.

его матричный элемент, отвечаю щий теореме.

удобство множителя $1/\sqrt{2J+1}$

по сути никогда не понимал, в чем это удобство состоит???

пример применения теоремы Вигнера-Эккарта

а хз, я не знаю.

О применениях (???)

(мб тут и укажу про правила отбора)

Сложение по Ландау

Полученное в §31 правило сложения моментов определяет возможные значения полного момента системы, состоящей из двух частиц (или более сложных частей), обладающих моментами j_1 и j_2[1]). Это правило в действительности тесно связано со свойствами волновых функций по отношению к пространственным вращениям и непосредственно следует из свойств спиноров. Волновые функции частиц с моментами j_1 и j_2 представляют собой симметричные спиноры рангов $2j_1$ и $2j_2$, а волновая функция системы дается их произведением

$$\psi^{(1)}\overbrace{\lambda\mu\cdots}^{2j_1}\psi^{(2)}\overbrace{\rho\sigma\cdots}^{2j_2}$$

Симметризуя это произведение по всем индексам, получим симметричный спинор ранга $2(j_1+j_2)$, отвечающий состоянию с полным моментом j_1+j_2. Далее, упростим произведение (106.1) по одной паре индексов, из которых один должен принадлежать $\psi^{(1)}$, а другой - $\psi^{(2)}$ (в противном случае получится нуль); при этом, в силу симметрии каждого из спиноров $\psi^{(1)}$ и $\psi^{(2)}$, безразлично, какие именно индексы берутся из $\lambda,\mu,...$, и $\rho,\sigma,...$ После симметризации получим симметричный спинор ранга $2(j_1+j_2-1)$, отвечающий состоянию с моментом j_1+j_2-1[2]).

Продолжая этот процесс, мы найдем в соответствии с известным уже нам правилом, что j пробегает значения от j_1+j_2 до $|j_1-j_2|$, причем каждое по одному разу. С математической точки зрения, речь идет здесь о разложении прямого произведения $D^{(j_1)}\times D^{(j_2)}$ двух неприводимых представлений группы вращений (с размерностями $2j_1+1$ и $2j_2+1$) на неприводимые части. В этих терминах правило сложения моментов записывается в виде разбиения

$$D^{(j_1)}\times D^{(j_2)}=D^{(j_1+j_2)}+D^{(j_1+j_2-1)}+...+D^{(|j_1-j_2|)}.$$

Для полного решения задачи о сложении моментов мы должны еще рассмотреть вопрос о составлении волновой функции системы с заданным значением полного момента по волновым функциям составляющих ее двух частиц.

Начнем с наиболее простого случая сложения двух моментов в равный нулю суммарный момент. При этом, очевидно, должно быть $j_1=j_2$, а проекции моментов $m_1=-m_2$. Пусть ψ_{jm} - нормированные волновые функции состояний одной частицы с моментом j и его проекцией m (в неспинорном представлении). Искомая волновая функция системы ψ_0 представляет собой сумму произведений волновых функций обеих частиц с противоположными значениями m:

$$\psi_0=\frac{1}{\sqrt{2j+1}}\sum_{m=-j}^{j}(-1)^{j-m}\psi^{(1)}_{jm}\psi^{(2)}_{j,-m}$$

(j- общее значение j_1 и j_2). Множитель перед суммой есть результат нормировки. Что касается коэффициентов в сумме, то все они должны быть одинаковы по своей абсолютной величине - уже в силу того, что все значения проекций m моментов частиц равновероятны. Порядок же чередования знаков в (106.2) легко найти с помощью спинорного представления волновых функций. В спинорных обозначениях сумма в (106.2) представляет собой скаляр (полный момент системы равен нулю!)

$$\psi^{(1)\lambda\mu...}\psi^{(2)}_{\lambda\mu...}$$

составленный из двух спиноров ранга $2j$. Заметив это, мы найдем знаки в (106.2) непосредственно из формулы (57.3).

Следует, однако, иметь в виду, что однозначными являются, вообще говоря, лишь относительные знаки членов суммы (106.2), общий же знак может оказаться зависящим от

«порядка сложения» моментов. Действительно, если опустить все спинорные индексы (среди которых $j+m$ единиц и $j-m$ двоек) у $\psi^{(1)}$ и поднять у $\psi^{(2)}$, то скаляр (106.3) умножится на $(-1)^{2j}$, т. е. при полуцелом j изменит знак.

Далее, рассмотрим систему с равным нулю полным моментом, составленную из трех частиц с моментами j_1, j_2, j_3 и их проекциями m_1, m_2, m_3. Условие равенства полного момента нулю подразумевает, что $m_1+m_2+m_3=0$, а j_1, j_2, j_3 имеют такие значения, что каждое из них может получиться в результате векторного сложения двух других, т.е. геометрически j_1, j_2, j_3 должны быть сторонами замкнутого треугольника; другими словами, каждое из них не меньше разности и не больше суммы двух других:

$$|j_1-j_2| \leqslant j_3 \leqslant j_1+j_2 \quad \text{и т. д.}$$

Очевидно, что алгебраическая сумма $j_1+j_2+j_3$ является при этом целым числом.

Волновая функция рассматриваемой системы имеет вид суммы

$$\psi_0 = \sum_{m_1 m_2 m_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \psi^{(1)}_{j_1 m_1} \psi^{(2)}_{j_2 m_2} \psi^{(3)}_{j_3 m_3},$$

взятой по значениям каждого из m_j в пределах от $-j_1$ до j_1. Коэффициенты в этой формуле называют $3j$-символами Вагнера. По определению, они отличны от нуля только при условии

$$m_1+m_2+m_3=0$$

При перестановке индексов $1,2,3$ волновая функция (106.4) может измениться лишь на несущественный фазовый множитель. Фактически $3j$-символы могут быть определены как чисто вещественные (см. ниже) и тогда неоднозначность ψ_0 может заключаться лишь в неопределенности ее общего знака (как это имеет место и для функции (106.2)). Это значит, что перестановка колонок $3j$-символа может либо оставлять его неизменным, либо менять его знак.

Наиболее симметричный способ определения коэффициентов в сумме (106.4), которым и принято определять $3j$-символы, заключается в следующем. В спинорных обозначениях ψ_0 представляет собой скаляр, составленный как произведение трех спиноров $\psi^{(1)\lambda\mu\cdots}, \psi^{(2)\lambda\mu\cdots}, \psi^{(3)\lambda\mu\cdots}$, упрощенное по всем парам индексов, каждая из которых относится к двум различным спинорам. Условимся, что в каждой паре, относящейся к частицам 1 и 2, спинорный индекс будет писаться сверху у $\psi^{(1)}$ и снизу у $\psi^{(2)}$; в паре, относящейся к частицам 2 и 3, - сверху у $\psi^{(2)}$ и снизу у $\psi^{(3)}$; в паре, относящейся к частицам 3 и 1, - сверху у $\psi^{(3)}$ и снизу у $\psi^{(1)}$ (легко подсчитать, что всего имеется соответственно $j_1+j_2-j_3, j_2+j_3-j_1$ и $j_1+j_3-j_2$ пар каждого из этих «сортов»). Этим правилом знак ψ_0 устанавливается однозначно. Очевидно, что при таком определении циклическая перестановка индексов $1,2,3$ оставляет ψ_0 неизменной. Это значит, что $3j$-символ не меняется при циклической перестановке его столбцов. Перестановка же двух (любых) индексов приведет, как легко сообразить, к необходимости поднять нижние и опустить верхние индексы во всех $j_1+j_2+j_3$ парах. Это значит, что ψ_0 умножится на $(-1)^{j_1+j_2+j_3}$; другими словами, $3j$-символы обладают свойством

$$\begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \quad \text{и т. д.},$$

т. е. меняют знак при перестановке двух колонок, если $j_1 + j_2 + +j_3$ - нечетное число. Наконец, легко видеть, что

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

Действительно, изменение знака z-компонент всех моментов может рассматриваться как результат поворота на угол π вокруг оси y. Но такое преобразование эквивалентно поднятию всех нижних и опусканию всех верхних спинорных индексов (cm. (58.5)).

От выражения (106.4) можно перейти к важной формуле, определяющей волновую функцию ψ_{jm} системы, состоящей из двух частиц и обладающей заданными значениями j и m. Для этого будем рассматривать совокупность частиц 1 и 2 как одну систему. Поскольку момент $\mathbf{j}$ этой системы вместе с моментом $\mathbf{j}_3$ частицы 3 складывается в равный нулю суммарный момент, должно быть $j = j_3, m = -m_3$. Согласно (106.2) можно тогда написать

$$\psi_0 = \frac{1}{\sqrt{2j+1}} \sum_m (-1)^{j-m} \psi_{jm} \psi^{(3)}_{j,-m}$$

Эту формулу надо сравнить с выражением (106.4) (в котором пишем $j, -m$ вместо j_3, m_3). При этом, однако, надо предварительно учесть, что правило составления суммы в (106.7) согласно (106.3) не соответствует правилу составления суммы (106.4): для приведения (106.7) к (106.4) надо, как легко сообразить, переставить верхние и нижние индексы в парах, соответствующих частицам 1 и 3; это приводит к появлению дополнительного множителя $(-1)^{j_1-j_2+j_3}$. В результате получим [1])

$$\psi_{jm} = (-1)^{j_1-j_2+m} \sqrt{2j+1} \sum_{m_1,m_2} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix} \psi^{(1)}_{j_1 m_1} \psi^{(2)}_{j_2 m_2}$$

где суммирование по m_1 и m_2 производится с учетом условия $m_1 + m_2 = m$

Формула (106.8) дает искомое разложение волновой функции системы по волновым функциям обеих частиц, обладающих определенными моментами j_1 и j_2. Ее можно записать в виде

$$\psi_{jm} = \sum_{m_1 m_2} \langle m_1 m_2 | jm \rangle \, \psi^{(1)}_{j_1 m_1} \psi^{(2)}_{j_2 m_2}, \quad m_2 = m - m_1.$$

Коэффициенты

$$\langle m_1 m_2 | jm \rangle = (-1)^{j_1-j_2+m} \sqrt{2j+1} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}$$

составляют матрицу преобразования от полной ортонормированной системы $(2j_1+1)(2j_2+1)$ волновых функций состояний $|m_1 m_2\rangle$ к такой же системе волновых функций состояний $|jm\rangle$ (при заданных значениях j_1, j_2). Их называют коэффициентами векторного сложения или коэффициентами Клебша-Гордана. Обозначение символом $\langle m_1 m_2 | jm \rangle$ соответствует общему способу обозначений коэффициентов разложения одной системы функций по другой согласно (11.18). Для упрощения записи мы опустили в этом символе совпадающие в обеих системах функций квантовые числа j_1, j_2; при необходимости эти числа включаются в обозначение: $\langle j_1 m_1 j_2 m_2 | j_1 j_2 jm \rangle^2$).

Матрица преобразования (106.9) унитарна (см. §12). Поэтому коэффициенты обратного преобразования

$$\psi^{(1)}_{j_1 m_1} \psi^{(2)}_{j_2 m_2} = \sum_{j=|j_2-j_1|}^{j_1+j_2} \langle j, m_1+m_2 | m_1 m_2 \rangle \, \psi_{j,m_1+m_2}$$

комплексно сопряжены с коэффициентами преобразования A06.9). Мы увидим ниже, что эти коэффициенты вещественны; поэтому просто

$$\langle m_1 m_2 | jm \rangle = \langle jm | m_1 m_2 \rangle \,.$$

Согласно общим правилам квантовой механики квадраты коэффициентов разложения (106.11) определяют вероятности системе иметь те или иные значения j, m (при заданных j_1, m_1 и j_2, m_2). Унитарность преобразования (106.9) означает, что его коэффициенты удовлетворяют определенным условиям ортогональности. Согласно формулам (12.5), (12.6) имеем

$$\begin{aligned}
&\sum_{m_1 m_2} \langle m_1 m_2 | jm \rangle \langle m_1 m_2 | j'm' \rangle = \\
=&(2j+1) \sum_{m_1, m_2} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j' \\ m_1 & m_2 & -m' \end{pmatrix} = \delta_{jj'} \delta_{mm'}, \\
&\sum_{j} \langle m_1 m_2 | jm \rangle \langle m_1' m_2' | jm \rangle = \\
&= \sum_{j} (2j+1) \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j \\ m_1' & m_2' & -m \end{pmatrix} = \delta_{m_1 m_1'} \delta_{m_2 m_2'}.
\end{aligned}$$

Явное общее выражение $3j$-символов довольно громоздко. Оно может быть представлено в виде [1])

$$\begin{aligned}
\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = &\left[\frac{(j_1+j_2-j_3)!\,(j_1-j_2+j_3)!\,(-j_1+j_2+j_3)!}{(j_1+j_2+j_3+1)!} \right]^{1/2} \times \\
\times &\left[(j_1+m_1)!\,(j_1-m_1)!\,(j_2+m_2)!\,(j_2-m_2)!\,(j_3+m_3)!\,(j_3-m_3)! \right]^{1/2} \times \\
&\times \sum_z \Big\{ [) - 1)^{z+j_1-j_2-m_3}] \left[z!\,(j_1+j_2-j_3-z)!\,(j_1-m_1-z)! \times \right. \\
&\left. \times (j_2+m_2-z)!\,(j_3-j_2+m_1+z)!\,(j_3-j_1-m_2+z)! \right]^{-1} \Big\} \,.
\end{aligned}$$

Суммирование производится по всем целым числам z; однако, поскольку факториал отрицательного числа равен ∞, число членов в сумме фактически конечно. Коэффициент перед суммой явно симметричен по индексам $1, 2, 3$; симметрия же суммы выявляется после соответствующего переобозначения переменной суммирования z.

Помимо свойств симметрии (106.5), (106.6), следующих простым образом из определения $3j$-символов, последние обладают еще и другими свойствами симметрии, вывод которых, однако, более сложен, и мы его здесь не приводим. Эти свойства удобно формулировать, если ввести квадратную (3×3) таблицу чисел, связанных с параметрами $3j$-символа следующим образом:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{bmatrix} j_2+j_3-j_1 & j_3+j_1-j_2 & j_1+j_2-j_3 \\ j_1-m_1 & j_2-m_2 & j_3-m_3 \\ j_1+m_1 & j_2+m_2 & j_3+m_3 \end{bmatrix}$$

(сумма чисел в каждой строке и каждом столбце этой таблицы равна $j_1+j_2+j_3$). Тогда: 1) перестановка любых двух столбцов таблицы умножает $3j$-символ на $(-1)^{j_1+j_2+j_3}$ (это свойство совпадает с (106.5)); 2) то же справедливо для перестановки любых двух строк (в отношении двух нижних строк это свойство совпадает с (106.6)); 3) 3j-символ не меняется при замене строк таблицы ее столбцами [1]).

Выпишем ряд более простых формул для некоторых частных случаев. Значение

$$\begin{pmatrix} j & j & 0 \\ m & -m & 0 \end{pmatrix} = (-1)^{j-m}\frac{1}{\sqrt{2j+1}}$$

соответствует формуле (106.2). Формулы

$$\begin{pmatrix} j_1 & j_2 & j_1+j_2 \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix} = (-1)^{j_1-j_2+m_1+m_2}\times$$
$$\times\left[\frac{(2j_1)!\,(2j_2)!\,(j_1+j_2+m_1+m_2)!\,(j_1+j_2-m_1-m_2)!}{(2j_1+2j_2+1)!\,(j_1+m_1)!\,(j_1-m_1)!\,(j_2+m_2)!\,(j_2-m_2)!}\right]^{1/2},$$
$$\begin{pmatrix} j_1 & j_2 & j_3 \\ j_1 & -j_1-m_3 & m_3 \end{pmatrix} = (-1)^{-j_1+j_2+m_2}\times$$
$$\times\left[\frac{(2j_1)!\,(-j_1+j_2+j_3)!\,(j_1+j_2+m_3)!\,(j_3-m_3)!}{(j_1+j_2+j_3+1)!\,(j_1-j_2+j_3)!\,(j_1+j_2-j_3)!\,(-j_1+j_2-m_3)!\,(j_3+m_3)!}\right]^{1/2}$$

получаются непосредственно из (106.14). Вывод же формулы

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix} = (-1)^p\left[\frac{(j_1+j_2-j_3)!(j_1-j_2+j_3)!(-j_1+j_2+j_3)!}{(2p+1)!}\right]^{1/2}\frac{p!}{(p-j_1)!(p-j_2)!(p-j_3)!},$$

где

$$2p = j_1+j_2+j_3$$

есть четное число, требует ряда дополнительных вычислений [1]) (при нечетном $2p$ этот $3j$-символ равен нулю в силу свойства симметрии (106.6)).

В табл. 9 приведены, для справок, значения $3j$-символов для $j_3 = 1/2, 1, 3/2, 2$. Для каждого j_3 указано минимальное число $3j$-символов, из которых с помощью соотношений (106.5), (106.6) можно получить остальные.

(тут большая таблица, ну и фиг с ней, не до нее, все равно чуть что сборник свойств углового момента буду открывать, если будет это нужно.)

ЛЛ-108.1

Определить угловую зависимость волновых функций частицы со спином $1/2$ в состояниях с заданными значениями орбитального момента l, полного момента j и его проекции m.

Р е ш е н и е.

Задача решается общей формулой (106.8), в которой надо под $\psi^{(1)}$ понимать собственные функции орбитального момента (т. е. сферические функции Y_{lm_l}), а под $\psi^{(2)}$ - спиновую волновую функцию $\chi(\sigma)$ (где $\sigma = \pm 1/2$):

$$\psi_{jm} = (-1)^{l+m-1/2}\sqrt{2j+1}\sum_\sigma \begin{pmatrix} l & 1/2 & j \\ m-\sigma & \sigma & -m \end{pmatrix} Y_{l,m-\sigma}\chi(\sigma).$$

Подставив значения $3j$-символов, получим

$$\psi_{l+1/2,m} = \sqrt{\frac{j+m}{2j}}\chi\left(\frac{1}{2}\right)Y_{l,m-1/2} + \sqrt{\frac{j-m}{2j}}\chi\left(-\frac{1}{2}\right)Y_{l,m+1/2},$$
$$\psi_{l-1/2,m} = -\sqrt{\frac{j-m+1}{2j+2}}\chi\left(\frac{1}{2}\right)Y_{l,m-1/2} + \sqrt{\frac{j+m+1}{2j+2}}\chi\left(-\frac{1}{2}\right)Y_{l,m+1/2}.$$

9.0.3 Matrix Elements of Tensors by Landau (?????)

Теория

В § 29 были получены формулы, определяющие зависимость матричных элементов векторной физической величины от значения проекции момента. Эти формулы являются в действительности частным случаем общих формул, решающих такую же задачу для неприводимого (см. с. 268) тензора любого ран Гa^1)

Совокупность $2k+1$ компонент неприводимого тензора ранга k(k - целое число) по своим трансформационным свойствам эквивалентна совокупности $2k+1$ сферических функций $Y_{kq}(q=-k,...,k)$ (см. примеч. на с. 268). Это значит, что путем составления соответствующих линейных комбинаций компонент тензора можно получить набор величин, преобразующихся при вращениях как функции Y_{kq}. Совокупность таких величин, которые мы будем обозначать здесь через f_{kq}, назовем сферическим тензором ранга k.

Так, вектору соответствует значение $k=1$, а величины f_{1q} связаны с компонентами вектора следующими формулами:

$$f_{10}=ia_z,\quad f_{1,\pm1}=\mp(i/\sqrt{2})\,(a_x\pm ia_y)$$

(ср. (57.7)). Аналогичные формулы для тензора второго ранга имеют вид

$$f_{20}=-\sqrt{3/2}a_{zz},\quad f_{2,\pm1}=\pm\,(a_{xz}\pm ia_{yz})\,,$$
$$f_{2,\pm2}=-(1/2)\,(a_{xx}-a_{yy}\pm 2ia_{xy})\,.$$

причем $a_{xx}+a_{yy}+a_{zz}=0$[1]). Составление тензорных произведений из двух (или большего числа) сферических тензоров $f_{k_1q_1}, f_{k_2q_2}$ происходит в соответствии с правилами сложения моментов, причем k_1, k_2 играют формально роль «моментов», соответствующих этим тензорам. Таким образом, из двух сферических тензоров рангов k_1 и k_2 можно образовать сферические тензоры рангов $K=k_1++k_2,...,|k_1-k_2|$ по формулам

$$(f_{k_1}g_{k_2})_{KQ}=\sum_{q_1q_2}\langle q_1q_2|KQ\rangle\, f_{k_1q_1}g_{k_2q_2}=$$
$$=(-1)^{k_1-k_2+Q}\sqrt{2K+1}\sum_{q_1q_2}\begin{pmatrix}k_1 & k_2 & K\\ q_1 & q_2 & -Q\end{pmatrix} f_{k_1q_1}g_{k_2q_2}$$

(ср. (106.9)). Скалярное произведение двух сферических тензоров одинакового ранга k принято, однако, определять как

$$(f_kg_k)_{00}=\sum_q(-1)^{k-q}f_{kq}g_{k,-q}$$

что отличается от определения по формуле (107.3) с $K=Q=0$ множителем $\sqrt{2k+1}$(ср. (106.2))[2]). Это определение можно представить также в виде

$$(f_kg_k)_{00}=\sum_q f_{kq}g^*_{kq},$$

если заметить, что комплексное сопряжение сферического тензора производится по правилу

$$f^*_{kq}=(-1)^{k-q}f_{k,-q}$$

ср. (28.9)[3]).

Представление физических величин в виде сферических тензоров в особенности удобно при вычислении их матричных элементов, так как позволяет воспользоваться для этой цели результатами теории сложения моментов. По определению матричных элементов, имеем

$$\widehat{f}_{kq}\psi_{njm} = \sum_{n'j'm'} \langle n'j'm' \,|f_{kq}|\, njm\rangle \, \psi_{n'j'm'},$$

где ψ_{njm} - волновые функции стационарных состояний системы, характеризуемых величиной ее момента j, его проекцией m и набором остальных квантовых чисел n. По своим трансформационным свойствам функции в правой и левой частях равенства (107.5)) соответствуют функциям в правой и левой частях равенства (106.11). Отсюда сразу следуют правила отбора.

Матричные элементы компонент f_{kq} неприводимого тензора ранга k отличны от нуля лишь для переходов $jm \to j'm'$, удовлетворяющих «правилу сложения моментов» $\mathbf{j}' = \mathbf{j} + \mathbf{k}$; при этом числа j', j, k должны удовлетворять «правилу треугольника» (т.е. могут измерять стороны замкнутого треугольника), а $m' = m + q$. В частности, диагональные матричные элементы могут быть отличны от нуля только при условии $2j \geqslant k$.

Далее, из той же трансформационной аналогии следует, что коэффициенты в сумме (107.5) должны быть пропорциональны коэффициентам в (106.11) (теорема Вагнера-Эккарта). Этим определяется зависимость коэффициентов от чисел m, m', в соответствии с чем представим матричные элементы в виде

$$\langle n'j'm' \,|f_{kq}|\, njm\rangle = i^k(-1)^{j_{\max}-m'} \begin{pmatrix} j' & k & j \\ -m' & q & m \end{pmatrix} \langle n'j' \,\|f_k\|\, nj\rangle$$

($j_{\max}$ - большее из чисел j и j'), где $\langle n'j' \,\|f_k\|\, nj\rangle$ - величины, не зависящие от m, m', q'; их называют приведенными матричными элементами. Эта формула решает поставленный вопрос об определении зависимости матричных элементов от проекций моментов. Эта зависимость оказывается полностью связанной со свойствами симметрии по отношению к группе вращений, между тем как зависимость от остальных квантовых чисел определяется уже физической природой самих величин f_{kq}[1]).

Операторы $\widehat{f}_{kq}$ связаны друг с другом соотношениями

$$\widehat{f}^{+}_{kq} = (-1)^{k-q}\widehat{f}_{k,-q}.$$

Поэтому для их матричных элементов имеет место равенство

$$\langle n'j'm' \,|f_{kq}|\, njm\rangle^* = (-1)^{k-q} \langle njm \,|f_{k,-q}|\, n'j'm'\rangle \,.$$

Подставив сюда (107.6) и воспользовавшись свойствами $3j$-символов (106.5), (106.6), получим для приведенных матричных элементов соотношение «эрмитовости» [1])

$$\langle n'j' \,\|f_k\|\, nj\rangle = \langle nj \,\|f_k\|\, n'j'\rangle^*$$

Матричные элементы скаляра (107.4) диагональны по j и m. Согласно правилу умножения матриц имеем

$$\langle n'jm \,|(f_k g_k)_{00}|\, njm\rangle = \\ = \sum_q (-1)^{k-q} \sum_{n''j''m''} \langle n'jm \,|f_{kq}|\, n''j''m''\rangle \, \langle n''j''m'' \,|g_{k,-q}|\, njm\rangle \,.$$

Подставив сюда выражения (107.6) и произведя суммирование по q и m'' с помощью соотношения ортогональности $3j$-символов (106.12), получим следующую формулу:

$$\langle n'jm \,|(f_k g_k)_{00}|\, njm\rangle = \frac{1}{2j+1} \sum_{n''j''} \langle n'j \,\|f_k\|\, n''j''\rangle \, \langle n''j'' \,\|g_k\|\, nj\rangle \,.$$

Аналогичным образом легко получить следующие формулы суммирования квадратов матричных элементов:

$$\sum_{qm'} |\langle n'j'm' | f_{kq} | njm\rangle|^2 = \frac{1}{2j+1} |\langle n'j' \| f_k \| nj\rangle|^2,$$
$$\sum_{mm'} |\langle n'j'm' | f_{kq} | njm\rangle|^2 = \frac{1}{2k+1} |\langle n'j' \| f_k \| nj\rangle|^2.$$

В первой из них суммирование производится по q и m' при заданном m, а во второй - по m и m' при заданном q (причем всегда $m' = m + q$)

Рассмотрим, со справочными целями, случай, когда величинами f_{kq} являются сами шаровые функции Y_{kq}, и дадим выражения их матричных элементов для переходов между состояниями одной частицы с целочисленными орбитальными моментами l_1 и l_2, т. е. интегралов

$$\langle l_1 m_1 | Y_{lm} | l_2 m_2\rangle = \int Y^*_{l_1 m_1} Y_{lm} Y_{l_2 m_2} do.$$

Помимо правила отбора, соответствующего правилу сложения моментов ($\mathbf{l} + \mathbf{l}_2 = \mathbf{l}_1$), для этих матричных элементов имеет место также правило, согласно которому сумма $l + l_1 + l_2$ должна быть четным числом. Оно связано с сохранением четности, в силу которого произведение четностей $(-1)^{l_1+l_2}$ обоих состояний должно совпадать с четностью $(-1)^l$ рассматриваемой физической величины (см. § 30).

Матричные элементы (107.13) являются частным случаем более общего интеграла, который будет вычислен в §110 (см. примеч. на с. 547). Они даются формулой

$$\langle l_1 m_1 | Y_{lm} | l_2 m_2\rangle = (-1)^{m_1} i^{-l_1+l_2+l} \begin{pmatrix} l_1 & l & l_2 \\ -m_1 & m & m_2 \end{pmatrix} \begin{pmatrix} l_1 & l & l_2 \\ 0 & 0 & 0 \end{pmatrix} \left[\frac{(2l+1)(2l_1+1)(2l_2+1)}{4\pi}\right]^{1/2}.$$

В частности, при $m_1 = m_2 = m = 0$ находим значение интеграла от произведения трех полиномов Лежандра

$$\int_{-1}^{1} P_l(\mu) P_{l_1}(\mu) P_{l_2}(\mu) d\mu = 2 \begin{pmatrix} l_1 & l & l_2 \\ 0 & 0 & 0 \end{pmatrix}^2$$

9.0.4 6j-Symbols by Landau

Теория

Мы определили в §106 $3j$-символы как коэффициенты в сумме (106.4), представляющей собой волновую функцию системы трех частиц с равным нулю полным моментом. С точки зрения трансформационных свойств по отношению к вращениям эта сумма является скаляром. Отсюда следует, что набор $3j$-символов с заданными значениями j_1, j_2, j_3 (и всеми возможными m_1, m_2, m_3) можно рассматривать как совокупность величин, преобразующихся при вращениях по закону, контраградиентному закону преобразования произведений $\psi_{j_1 m_1} \psi_{j_2 m_2} \psi_{j_3 m_3}$ - так, чтобы обеспечить инвариантность всей суммы.

В связи с такой точкой зрения можно поставить вопрос о построении скаляра, составленного из одних только $3j$-символов. Такой скаляр должен зависеть только от чисел j, но не от чисел m, меняющихся при вращениях. Другими словами, он должен выражаться в виде сумм по всем числам m. Каждое такое суммирование состоит в

«упрощении» произведения двух $3j$-символов по правилу

$$\sum_m (-1)^{j-m} \begin{pmatrix} j.. \\ m.. \end{pmatrix} \begin{pmatrix} j.. \\ -m.. \end{pmatrix}$$

(ср. способ составления скаляра (106.2)).

Поскольку в каждом «упрощении» фигурирует пара чисел m, для составления полного скаляра надо рассматривать произведения четного числа $3j$-символов. Упрощение произведения двух $3j$-символов приводит, в силу свойства их ортогональности, к тривиальному результату:

$$\sum_{m_1 m_2 m_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} \times$$

$$\times (-1)^{j_1+j_2+j_3-m_1-m_2-m_3} = \sum_{m_1 m_2 m_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}^2 = 1$$

(здесь использовано равенство $m_1 + m_2 + m_3 = 0$ и формулы (106.6) и (106.12)). Поэтому наименьшее число сомножителей, необходимое для получения нетривиального скаляра, равно четырем. В каждом $3j$-символе три числа j составляют геометрически замкнутый треугольник. Поскольку каждое число j должно фигурировать, при «упрощении», в двух $3j$-символах, то ясно, что при составлении скаляра из произведений четырех $3j$-символов имеется 6 чисел j, которые геометрически должны изображаться длинами ребер неправильного тетраэдра (рис. 45); каждому из $3j$-символов соответствует одна из его граней. В определении искомого скаляра принято определенное условие в отношении произведения процесса упрощения, выражаемое следующей формулой:

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = \sum_{\text{все } m} (-1)^{\sum_i^{i(j_i - m_i)}} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} \times$$

$$\times \begin{pmatrix} j_1 & j_5 & j_6 \\ m_1 & -m_5 & m_6 \end{pmatrix} \begin{pmatrix} j_4 & j_2 & j_6 \\ m_4 & m_2 & -m_6 \end{pmatrix} \begin{pmatrix} j_4 & j_5 & j_3 \\ -m_4 & m_5 & m_3 \end{pmatrix}$$

Суммирование производится здесь по всем возможным значениям всех чисел m; поскольку, однако, сумма трех m в каждом $3j$-символе должна быть равна нулю, фактически лишь три из шести m независимы. Величины, определенные формулой (108.2), называют $6j$-символами или коэффициентами *Рака*[1]).

Из определения (108.2), с учетом свойств симметрии $3j$-символов, легко убедиться в том, что $6j$-символ не меняется при Рис. 45 любой перестановке трех его столбцов, а в каждой паре столбцов можно переставить верхнее и нижнее числа. В силу этих свойств симметрии последовательность чисел $j_1 \ldots j_6$ в $6j$-символе можно представить в 24 эквивалентных видах [2]). Кроме того, $6j$-символы обладают еще одним, менее очевидным, свойством симметрии, устанавливающим равенство между символами с различными наборами чисел j:

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = \begin{Bmatrix} j_1 & \frac{1}{2}(j_2 + j_5 + j_3 - j_6) & \frac{1}{2}(j_3 + j_6 + j_2 - j_5) \\ j_4 & \frac{1}{2}(j_2 + j_5 + j_6 - j_3) & \frac{1}{2}(j_3 + j_6 + j_5 - j_2) \end{Bmatrix}$$

(T. Regge, 1959) Укажем полезное соотношение между $6j$ - и $3j$-символами, которое можно получить с помощью определения (108.2):

$$\sum_{m_4 m_5 m_6} (-1)^{j_4+j_5+j_6-m_4-m_5-m_6} \begin{pmatrix} j_1 & j_5 & j_6 \\ m_1 & -m_5 & m_6 \end{pmatrix} \begin{pmatrix} j_4 & j_2 & j_6 \\ m_4 & m_2 & -m_6 \end{pmatrix} \times$$

$$\times \begin{pmatrix} j_4 & j_5 & j_3 \\ -m_4 & m_5 & m_3 \end{pmatrix} = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix}. \quad (108.4)$$

Выражение, суммируемое в левой части равенства, отличается от суммы в (108.2), отсутствием одного множителя (3j-символа). Можно сказать поэтому, что сумма в (108.4) изображается тетраэдром (рис. 45) без одной из его граней; этим определяется отличие суммы от скаляра. Другими словами, по своим трансформационным свойствам она соответствует одному $3j$-символу - стоящему в правой части равенства (108.4), которому она должна быть пропорциональна. Коэффициент же пропорциональности ($6j$-символ в правой части равенства) легко получить, умножив обе части равенства на

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

и просуммировав по оставшимся числам m_1, m_2, m_3. $6j$-символы появляются естественным образом при рассмотрении следующего вопроса, связанного со сложением трех моментов.

Пусть три момента j_1, j_2, j_3 складываются в результирующий момент J. Заданием момента J (и его проекции M) состояние системы, однако, еще не определяется однозначным образом; оно зависит и от способа сложения моментов (или, как говорят, от схемы их связи).

Рассмотрим, например, такие две схемы связи: 1) сначала моменты j_1 и j_2 складываются в суммарный момент j_{12}, а затем j_{12} и j_3 складываются в окончательный момент J; 2) моменты j_2 и j_3 складываются в j_{23}, а затем j_{23} и j_1 - в J. Первой схеме соответствуют состояния, в которых (наряду с $j_1, j_2 j_3,\ J, M$) имеет определенное значение величина j_{12}; их волновые функции обозначим через $\psi_{j_{12}JM}$ (опуская, для краткости, повторяющиеся индексы $j_1 j_2 j_3$). Аналогично, волновые функции второй схемы связи обозначим через $\psi_{j_{23}JM}$ В обоих случаях значения «промежуточного» момента (j_{12} или j_{23}), вообще говоря, неоднозначны, так что мы имеем (при заданных J, M) два различных набора состояний, различающихся значениями j_{12} или j_{13}. Согласно общим правилам функции этих двух наборов связаны друг с другом определенным унитарным преобразованием

$$\psi_{j_{23}JM} = \sum_{j_{12}} \langle j_{12}|j_{23}\rangle\, \psi_{j_{12}JM}$$

Из физических соображений очевидно, что коэффициенты этого преобразования не зависят от числа M - они не могут зависеть от ориентации всей системы в пространстве. Таким образом, они зависят лишь от значений шести моментов лярными (в указанном выше смысле) величинами. Фактическое вычисление этих коэффициентов легко произвести следующим образом. Путем двукратного применения формулы (106.9) находим

$$\begin{aligned}\psi_{j_{23}JM} &= \sum_{(m)} \langle m_1 m_{23}|JM\rangle\, \psi_{j_1 m_1}\psi_{j_{23}m_{23}} = \\ &= \sum_{(m)} \langle m_1 m_{23}|JM\rangle\, \langle m_2 m_3|j_{23}m_{23}\rangle\, \psi_{j_1 m_1}\psi_{j_2}m_2\psi_{j_3 m_3}, \\ \psi_{j_{12}JM} &= \sum_{(m)} \langle m_3 m_{12}|JM\rangle\, \langle m_1 m_2|j_{12}m_{12}\rangle\, \psi_{j_1 m_1}\psi_{j_2 m_2}\psi_{j_3 m_3}\end{aligned}$$

(знак (m) под знаком суммы означает, что суммирование производится по всем входящим в выражение числам $m_1, m_2, \ldots$). Используя ортонормированность функций ψ_{jm}, найдем теперь

$$\begin{aligned}&\langle j_{12}|j_{23}\rangle \equiv \int \psi^*_{j_{12}JM}\psi_{j_{23}JM}dq = \\ &= \sum_{(m)} \langle m_3 m_{12}|JM\rangle\, \langle m_1 m_{23}|JM\rangle\, \langle m_1 m_2|j_{12}m_{12}\rangle\, \langle m_2 m_3|j_{23}m_{23}\rangle\,.\end{aligned}$$

Сумма в правой части равенства берется при заданном значении M, но результат суммирования в действительности (по указанной выше причине) от M не зависит. Поэтому суммирование можно распространить и по значениям M, введя при этом перед суммой множитель $1/(2J+1)$. Выражая затем коэффициенты $\langle m_1 m_2|jm\rangle$ через $3j$-символы согласно (106.10), получим:

$$\langle j_{12}|j_{23}\rangle = (-1)^{j_1+j_2+j_3+J}\sqrt{(2j_{12}+1)\,(2j_{23+1})}\left\{\begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & J & j_{23}\end{array}\right\}.$$

Связь $6j$-символов с коэффициентами преобразования (108.5) позволяет легко получить некоторые полезные формулы для суммирования произведений $6j$-символов.

Прежде всего, в силу унитарности преобразования (108.5) (и вещественности его коэффициентов), имеет место соотношение

$$\sum_j (2j+1)\,(2j''+1)\left\{\begin{array}{ccc} j_1 & j_2 & j' \\ j_3 & j_4 & j\end{array}\right\}\left\{\begin{array}{ccc} j_3 & j_2 & j \\ j_1 & j_4 & j''\end{array}\right\} = \delta_{j'j''}$$

Далее рассмотрим три схемы связи трех моментов-с промежуточными суммами соответственно j_{12}, j_{23} и j_{31}. Коэффициенты соответствующих преобразований (108.6) связаны между собой, согласно правилу умножения матриц, соотношением

$$\sum_{j_{23}} \langle j_{12}|j_{23}\rangle\,\langle j_{23}|j_{31}\rangle = \langle j_{12}|j_{31}\rangle$$

Подставив сюда (108.6) и изменив обозначение индексов, получим

$$\sum_j (-1)^{j+j_3+j_6}(2j+1)\left\{\begin{array}{ccc} j_2 & j_4 & j_6 \\ j_1 & j_5 & j\end{array}\right\}\left\{\begin{array}{ccc} j_4 & j_1 & j_6 \\ j_2 & j_5 & j_3\end{array}\right\} = \left\{\begin{array}{ccc} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6\end{array}\right\}.$$

Наконец, путем рассмотрения различных схем связи четырех моментов можно получить [1]) следующую формулу сложения для произведений трех $6j$-символов:

$$\sum_j (-1)^{j+\sum_1^9 j_i}(2j+1)\left\{\begin{array}{ccc} j_4 & j_2 & j_6 \\ j_9 & j_8 & j\end{array}\right\}\left\{\begin{array}{ccc} j_2 & j_1 & j_3 \\ j_7 & j & j_9\end{array}\right\}\left\{\begin{array}{ccc} j_4 & j_3 & j_5 \\ j_7 & j_8 & j\end{array}\right\} =$$
$$= \left\{\begin{array}{ccc} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6\end{array}\right\}\left\{\begin{array}{ccc} j_6 & j_1 & j_5 \\ j_7 & j_8 & j_9\end{array}\right\} \quad (108.9)$$

(L. C. Biedenharn, J. P. Elliott, 1953). Приведем, для справок, некоторые явные выражения для $6j$-символов. $6j$-символ может быть представлен в общем случае в виде следующей суммы:

$$\left\{\begin{array}{ccc} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6\end{array}\right\} = \Delta\,(j_1 j_2 j_3)\,\Delta\,(j_1 j_5 j_6)\,\Delta\,(j_4 j_2 j_6)\,\Delta\,(j_4 j_5 j_3)\times$$
$$\times \sum_z \frac{(-1)^z (z+1)!}{(z-j_1-j_2-j_3)!\,(z-j_1-j_5-j_6)!\,(z-j_4-j_2-j_6)!\,(z-j_4-j_5-j_3)!}\times$$
$$\times\,(j_1+j_2+j_4+j_5-z)!\,(j_2+j_3+j_5+j_6-z)!\,(j_3+j_1+j_6+j_4-z)!$$

где

$$\Delta(abc) = \left[\frac{(a+b-c)!(a-b+c)!(-a+b+c)!}{(a+b+c+1)!}\right],$$

а сумма берется по всем положительным целым значениям z, при которых ни один из факториалов в знаменателе не имеет отрицательного аргумента. В табл. 10 даны

формулы $6j$-символов для случаев, когда один из параметров равен $0, 1/2$ или 1. В заключение сделаем несколько замечаний о составляемых из $3j$-символов скалярах более высокого порядка.

Следующим по сложности после $3j$-символа является скаляр, составляемый путем упрощения произведений шести $3j$-символов. Эти $3j$-символы содержат 18 попарно совпадающих чисел j, так что возникающий в результате скаляр зависит от 9 параметров j. Его принято называть $9j$-символом и определять следующим образом (E. Wigner, 1951):

$$\left\{ \begin{array}{ccc} j_{11} & j_{12} & j_{13} \\ j_{21} & j_{22} & j_{23} \\ j_{31} & j_{32} & j_{33} \end{array} \right\} = \sum_{\text{все } m} \left(\begin{array}{ccc} j_{11} & j_{12} & j_{13} \\ m_{11} & m_{12} & m_{13} \end{array} \right) \left(\begin{array}{ccc} j_{21} & j_{22} & j_{23} \\ m_{21} & m_{22} & m_{23} \end{array} \right) \times$$
$$\times \left(\begin{array}{ccc} j_{31} & j_{32} & j_{33} \\ m_{31} & m_{32} & m_{33} \end{array} \right) \left(\begin{array}{ccc} j_{11} & j_{21} & j_{31} \\ m_{11} & m_{21} & m_{31} \end{array} \right) \times$$
$$\times \left(\begin{array}{ccc} j_{12} & j_{22} & j_{32} \\ m_{12} & m_{22} & m_{32} \end{array} \right) \left(\begin{array}{ccc} j_{13} & j_{23} & j_{33} \\ m_{13} & m_{23} & m_{33} \end{array} \right) \cdot \quad (108.11)$$

(тут таблица еще, ее тоже не пишу, потому что не нужна она вообще)

Эта величина может быть также представлена в виде суммы произведений трех $6j$-символов:

$$\left\{ \begin{array}{ccc} j_{11} & j_{12} & j_{13} \\ j_{21} & j_{22} & j_{23} \\ j_{31} & j_{32} & j_{33} \end{array} \right\} = \sum_j (-1)^{2j} (2j+1) \left\{ \begin{array}{ccc} j_{11} & j_{21} & j_{31} \\ j_{32} & j_{33} & j \end{array} \right\} \times$$
$$\times \left\{ \begin{array}{ccc} j_{12} & j_{22} & j_{32} \\ j_{21} & j & j_{23} \end{array} \right\} \left\{ \begin{array}{ccc} j_{13} & j_{23} & j_{33} \\ j & j_{11} & j_{12} \end{array} \right\}.$$

В эквивалентности (108.11) и (108.12) можно убедиться, подставив в (108.12) определение (108.2) и воспользовавшись свойствами ортогональности $3j$-символов. $9j$-символ обладает высокой симметрией, следующей непосредственно из определения (108.11) и свойств симметрии $3j$-символов. Легко убедиться, что при перестановке любых его двух строк или двух столбцов $9j$-символ умножается на $(-1)^{\Sigma j}$. Кроме того, $9j$-символ не меняется при транспонировании, т.е. при взаимной замене строк и столбцов.

Скаляры еще более высоких порядков зависят от еще большего числа параметров j. Очевидно, что это число должно быть всегда кратно трем ($3nj$-символы). Мы не будем останавливаться здесь на свойствах этих величин. Упомянем лишь, что при каждом $n > 3$ имеется более чем по одному различному не сводящемуся друг к другу типу $3nj$-символов. Так, имеется два различных типа $12j$-символов [1]).

9.0.5 Matrix Elements in the Addition of Momenta by Landau (!!!)

(!!! а вот это очень важно проработать, выше уже были про это темы)

Теория

Рассмотрим снова систему, состоящую из двух частей (о которых будем говорить как о подсистемах 1 и 2), и пусть $f^{(1)}_{kq}$ сферический тензор, характеризующий первую из них. Его матричные элементы по отношению к волновым функциям этой же подсистемы определяются, согласно (107.6), формулой

$$\left\langle n'_1 j'_1 m'_1 \left| f^{(1)}_{kq} \right| n_1 j_1 m_1 \right\rangle = i^k (-1)^{j_1 \max - m'_1} \left(\begin{array}{ccc} j'_1 & k & j_1 \\ -m'_1 & q & m_1 \end{array} \right) \left\langle n'_1 j'_1 \left\| f^{(1)}_k \right\| n_1 j_1 \right\rangle$$

Возникает вопрос о вычислении матричных элементов этих же величин по отношению к волновым функциям системы в целом; покажем, как они могут быть выражены через те же приведенные матричные элементы, которые фигурируют в выражениях (109.1).

Состояния системы в целом определяются квантовыми числами $j_1 j_2 JM n_1 n_2 (J, M$ - величина и проекция момента всей системы). Поскольку $f^{(1)}_{kq}$ относится к подсистеме 1, ее оператор коммутирует с оператором момента подсистемы 2. Поэтому ее матрица диагональна по j_2; она диагональна также и по остальным квантовым числам n_2 этой подсистемы. Эти индексы (j_2, n_2) мы будем для краткости опускать и будем писать искомые матричные элементы в виде

$$\left\langle n'_1 j'_1 J' M' \left| f^{(1)}_{kq} \right| n_1 j_1 J M \right\rangle$$

Согласно (107.6) их зависимость от числа M определяется формулой

$$\left\langle n'_1 j'_1 J' M' \left| f^{(1)}_{kq} \right| n_1 j_1 J M \right\rangle = i^k (-1)^{J_{\max} - M'} \begin{pmatrix} J' & k & J \\ -M' & q & M \end{pmatrix} \left\langle n'_1 j'_1 J' \left\| f^{(1)}_{k} \right\| n_1 j_1 J \right\rangle .$$

Для установления связи между приведенными матричными элементами в правых частях (109.1) и (109.2) пишем, по определению матричных элементов:

$$\begin{aligned} &\left\langle n'_1 j'_1 J' M' \left| f^{(1)}_{kq} \right| n_1 j_1 J M \right\rangle = \int \psi^*_{J'M'} \widehat{f}^{(1)}_{kq} \psi_{JM} dq = \\ &= \sum_{m_1 m'_1} (-1)^{j'_1 - j_2 + M' - M} \sqrt{(2J'+1)(2J+1)} \begin{pmatrix} j'_1 & j_2 & J' \\ m'_1 & m_2 & -M' \end{pmatrix} \times \\ &\times \begin{pmatrix} j_1 & j_2 & J \\ m_1 & m_2 & -M \end{pmatrix} \left\langle n'_1 j'_1 m'_1 \left| f^{(1)}_{kq} \right| n_1 j_1 m_1 \right\rangle . \end{aligned}$$

Подставив сюда (109.1), (109.2) и сравнив полученное соотношение с формулой (108.4), мы увидим, что отношение приведенных матричных элементов (в (109.1), (109.2)) должно быть пропорционально определенному $6j$-символу. Тщательное сравнение обоих указанных соотношений приводит к следующей окончательной формуле:

$$\begin{aligned} \left\langle n'_1 j'_1 J' \left\| f^{(1)}_{k} \right\| n_1 j_1 J \right\rangle =& (-1)^{j_{1\max} + j_2 + J_{\min} + k} \sqrt{(2J+1)(2J'+1)} \times \\ &\times \begin{Bmatrix} j'_1 & J' & j_2 \\ J & j_1 & k \end{Bmatrix} \left\langle n'_1 j'_1 \left\| f^{(1)}_{k} \right\| n_1 j_1 \right\rangle \end{aligned} \quad (109.3)$$

(здесь $j_{1\max}$ - большее из j_1, j'_1; $J_{\min}$ - меньшее из J, J'). Аналогичная формула для приведенных матричных элементов сферического тензора, относящегося к второй подсистеме:

$$\begin{aligned} \left\langle n'_2 j'_2 J' \left\| f^{(2)}_{k} \right\| n_2 j_2 J \right\rangle =& (-1)^{j_1 + j_{2\min} + J_{\max} + k} \sqrt{(2J+1)(2J'+1)} \times \\ &\times \begin{Bmatrix} j'_2 & J' & j_1 \\ J & j_2 & k \end{Bmatrix} \left\langle n'_2 j'_2 \left\| f^{(2)}_{k} \right\| n_2 j_2 \right\rangle . \end{aligned} \quad (109.4)$$

Отсутствие полной симметрии между выражениями (109.3) и (109.4) (в показателе степени у -1) связано с зависимостью фазы волновых функций от порядка сложения моментов. Эту разницу надо иметь в виду, если приходится вычислять матричные элементы одновременно для обеих подсистем.

Далее, найдем полезную формулу для матричных элементов по отношению к волновым функциям всей системы от скалярного произведения (см. определение (107.4))

двух сферических тензоров одинакового ранга k, относящихся к различным подсистемам (и потому коммутирующих друг с другом). Согласно (107.10) эти матричные элементы выражаются через приведенные матричные элементы каждого из тензоров (по отношению к волновым функциям системы в целом) следующим обраЗом:

$$\left\langle n_1' n_2' j_1' j_2' JM \left| \left(f_k^{(1)} f_k^{(2)} \right)_{00} \right| n_1 n_2 j_1 j_2 JM \right\rangle =$$

$$= \frac{1}{2J+1} \sum_{J''} \left\langle n_1' j_1' J \left\| f_k^{(1)} \right\| n_1 j_1 J'' \right\rangle \left\langle n_2' j_2' J'' \left\| f_k^{(2)} \right\| n_2 j_2 J \right\rangle$$

(здесь использовано, что матрица величины, относящейся к одной из подсистем, диагональна по квантовым числам другой подсистемы). Подставив сюда (109.3), (109.4) и воспользовавшись формулой суммирования (108.8), получим искомую формулу, выражающую матричные элементы скалярного произведения через приведенные матричные элементы каждого из тензоров по отношению к волновым функциям соответствующих подсистем:

$$\left\langle n_1' n_2' j_1' j_2' JM \left| \left(f_k^{(1)} f_k^{(2)} \right)_{00} \right| n_1 n_2 j_1 j_2 JM \right\rangle =$$

$$= (-1)^{j_1 \min + j_2 \max + J} \left\{ \begin{array}{ccc} J & j_2' & j_1' \\ k & j_1 & j_2 \end{array} \right\} \left\langle n_1' j_1' \left\| f_k^{(1)} \right\| n_1 j_1 \right\rangle \left\langle n_2' j_2' \left\| f_k^{(2)} \right\| n_2 j_2 \right\rangle .$$

9.0.6 Matrix Elements for Axially Symmetric Systems by Landau

Теория

Основой для вычисления матричных элементов величин, характеризующих системы типа симметричного волчка, служит выражение интеграла от произведения трех D-функций.

Для вывода этой формулы вернемся к разложению (106.11)

$$\psi_{j_1 m_1} \psi_{j_2 m_2} = \sum_j \langle jm | m_1 m_2 \rangle \, \psi_{jm}, \quad m = m_1 + m_2$$

и преобразуем обе части равенства конечным поворотом системы координат. Каждая из ψ-функций преобразуется согласно (58.7), так что получим

$$\sum_{m_1' m_2'} D^{(j_1)}_{m_1' m_1} D^{(j_2)}_{m_2' m_2} \psi_{j_1 m_1'} \psi_{j_2 m_2'} = \sum_j \sum_m \langle jm | m_1 m_2 \rangle \, D^{(j)}_{m' m} \psi_{jm'}$$

Выразив теперь функции $\psi_{jm'}$ в правой части равенства в виде разложения (106.9) и сравнив коэффициенты при одинаковых произведениях $\psi_{j_1 m_1}, \psi_{j_2 m_2}$, получим соотношения

$$D^{(j_1)}_{m_1' m_1}(\omega) D^{(j_2)}_{m_2' m_2}(\omega) = \sum_j \langle m_1' m_2' | jm' \rangle \, D^{(j)}_{m' m}(\omega) \, \langle m_1 m_2 | jm \rangle$$

(причем $m = m_1 + m_2, m' = m_1' + m_2'$, а ω обозначает совокупность трех эйлеровых углов α, β, γ. Выраженная через $3j$-символы, эта формула принимает вид

$$D^{(j_1)}_{m_1' m_1}(\omega) D^{(j_2)}_{m_2' m_2}(\omega) = \sum_j (2j+1) \begin{pmatrix} j_1 & j_2 & j \\ m_1' & m_2' & -m' \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix} D^{(j)*}_{-m', -m}(\omega)$$

(здесь использовано также свойство D-функций (58.19)).

Умножив равенство (110.2) с обеих сторон на $D^{(j)}_{-m',-m}(\omega)$ и проинтегрировав его по $d\omega$ с помощью соотношения ортогональности (58.20), получим

$$\int D^{(j_1)}_{m'_1 m_1}(\omega) D^{(j_2)}_{m'_2 m_2}(\omega) D^{(j_3)}_{m'_3 m_3}(\omega) \frac{d\omega}{8\pi^2} = \begin{pmatrix} j_1 & j_2 & j_3 \\ m'_1 & m'_2 & m'_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

(для большей симметрии здесь произведено очевидное изменение обозначений индексов). Это и есть искомая формула [1]).

Пусть $f_{kq'}$ - сферический тензор ранга k, характеризующий волчок в связанных с ним координатных осях $x'y'z' \equiv \xi\eta\zeta$ (ось ζ - по оси волчка); это может быть, например, тензор мультипольного электрического или магнитного момента. Пусть f_{kq} - компоненты того же тензора относительно неподвижных осей координат xyz. Связь между теми и другими определяется матрицей конечных вращений согласно

$$f_{kq} = \sum_{q'} D^{(k)}_{q'q}(\omega) f_{kq'}$$

Волновые функции, описывающие вращение системы как целого, отличаются от D-функций лишь нормировкой:

$$\psi_{jm\mu} = i^j \sqrt{\frac{2j+1}{8\pi^2}} D^{(j)}_{\mu m}(\omega)$$

где j - полный момент системы; m - его проекция на неподвижную ось z; μ-проекция на ось системы; фазовый множитель выбран так, чтобы при целочисленном j и $\mu = 0$ функция (110.5) переходила в собственную функцию свободного момента (ср. (103.8)). Вычисляя по этим функциям матричный элемент величины (110.4) с помощью (110.3) (причем комплексно сопряженная D-функция выражается согласно (58.19)), получим

$$\langle j'\mu'm' \,|f_{kq}|\, j\mu m\rangle = i^{j-j'}(-1)^{\mu'-m'} \sqrt{(2j+1)(2j'+1)} \begin{pmatrix} j' & k & j \\ -\mu' & q' & \mu \end{pmatrix} \begin{pmatrix} j' & k & j \\ -m' & q & m \end{pmatrix} \langle \mu' \,|f_{kq'}|\, \mu\rangle$$
$$(\text{причем } \; q' = \mu' - \mu, q = m' - m)\,.$$

Эта формула решает поставленную задачу. Она определяет зависимость матричных элементов от моментов j, j' и их проекций m, m'. Что касается зависимости от квантовых чисел μ, μ', то она остается, разумеется, неопределенной: значения этих чисел зависят от «внутренних» состояний системы, между которыми берется «внутренний» матричный элемент $\langle \mu' \,|f_{kq'}|\, \mu\rangle$. Зависимость матричных элементов (110.6) от чисел m, m', такая же, как для всякой системы с заданным полным моментом. Отделив эту зависимость введением приведенных матричных элементов согласно (107.6), получим для последних выражение

$$\langle j'\mu' \,\|f_k\|\, j\mu\rangle = i^{j-j'-k}(-1)^{j_{\max}-\mu'} \sqrt{(2j+1)(2j'+1)} \begin{pmatrix} j' & k & j \\ -\mu' & q' & \mu \end{pmatrix} \langle \mu' \,|f_{kq'}|\, \mu\rangle\,.$$

Квадрат модуля матричного элемента (110.6), просуммированный по всем значениям конечного числа m' (и по $q = m' - m$) при заданном m, не зависит от значения m и равен, по общему правилу (107.11):

$$\sum_{qm'} |\langle j'\mu'm' \,|f_{kq}|\, j\mu m\rangle|^2 = \frac{1}{2j+1} |\langle j'\mu' \,\|f_k\|\, j\mu\rangle|^2 = (2j'+1) \begin{pmatrix} j' & k & j \\ -\mu' & q' & \mu \end{pmatrix}^2 |\langle \mu' \,|f_{kq'}|\, \mu\rangle|^2$$

Соотношения эрмитовости (107.9) для приведенных матричных элементов в координатах xyz(110.7), как и следовало, находятся в согласии с соотношениями (107.8)

$$\langle \mu \,|f_{kq'}|\, \mu\rangle = (-1)^{k-q} \langle \mu \,|f_{k,-q'}|\, \mu'\rangle^*$$

для матричных элементов в координатах $\xi\eta\zeta$. Вращение таких аксиально-симметричных систем, как двухатомная молекула (или аксиальное ядро), описывается всего двумя углами ($\alpha \equiv \varphi, \beta \equiv \theta$), определяющими направление оси системы. Вращательная волновая функция отличается в этом случае от (110.5) отсутствием множителя $e^{i\mu\gamma}/\sqrt{2\pi}$ (ср. примеч. на с. 389). Это изменение, однако, не отражается на матричных элементах: поскольку зависимость $D^{(j)}_{m'm}(\alpha,\beta,\gamma)$ от γ сводится к множителю $e^{im'\gamma}$, то (110.3) можно переписать в виде

$$\delta_{m'0} \int D^{(j_1)}_{m'_1 m_1}(\alpha,\beta,0) D^{(j_2)}_{m'_2 m_2}(\alpha,\beta,0) D^{(j_3)}_{m'_3 m_3}(\alpha,\beta,0) \frac{\sin\alpha d\alpha d\beta}{4\pi} = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m'_1 & m'_2 & m'_3 \end{pmatrix}$$

(где $m' = m'_1 + m'_2 + m'_3$) и результат вычисления интеграла не меняется. При этом правило отбора по проекции момента на ось системы соблюдается в прежнем виде ($\mu' - \mu = q'$), возникая (как следствие симметрии молекулы относительно оси ζ) в результате ортогональности электронных волновых функций. В формулах (110.6), (110.7) под $\langle \mu' \,|f_{kq'}|\, \mu\rangle$ надо понимать теперь матричные элементы по отношению к электронным состояниям при неподвижных ядрах.

9.0.7 Other About Addition of Momenta

(тут много можно дополнений найти, некоторые укажу.)

Электрон находится в двух состояниях одновременно

(тут с формулами это и покажу, это мы и видим.)

В задаче про сложение моментов проявляется принцип суперпозиции

(тут и укажу это)

О возможных классических аналогиях (??)

(их тоже придумать можно много.)

10 Other Template Models and Basic Special Method

10.1 Motion in a magnetic field

(??!! а я то думал, чего так плохо задачи решаются, теорию ведь всё еще не написал!)

10.1.1 Description of Motion in Magnetic Field by Landau (?)

(у него в книге много про это теории, мне очень лень ее смотреть, надеюсь, что не особо оно нужно.)

10.1.2 Landau Levels

Обсудим подробно уровни Ландау.

10.1.3 Degeneracy of Landau Levels

(добавлю часть параграфа из ЛЛ3, так это и понимаю)

Кратность уровней Ландау в особых ситуациях

(???? если у нас не кубик, то как считать кратность??? пока оставил вопрос, вряд ли думать про это актуально)

10.1.4 2.1. Pauli Hamiltonian by Tahtajan

The classical particle of charge e moving in the electromagnetic field with the vector potential $\boldsymbol{A}(\boldsymbol{x})$ and the scalar potential $\varphi(\boldsymbol{x})$ is described by the Hamiltonian function

$$H_{\mathrm{c}}(\boldsymbol{p},\boldsymbol{x})=\frac{1}{2m}\left(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A}\right)^2+e\varphi(\boldsymbol{x}),\quad \boldsymbol{x}=(x,y,z)\in\mathbb{R}^3$$

(see Problem 1.27 in Section 1.7 of Chapter 1). As we have seen in Example 2.3 in Section 2.4 of Chapter 2, the corresponding Hamiltonian operator of the spinless particle is given by

$$H^0=\frac{1}{2m}\left(\boldsymbol{P}-\frac{e}{c}\boldsymbol{A}\right)^2+e\varphi(\boldsymbol{x}). \tag{2.1}$$

However, quantum particles with spin interact with the magnetic field, so that the Hamiltonian H^0, which is an operator in the Hilbert space $\mathscr{H}=$
$L^2\left(\mathbb{R}^3,d^3\boldsymbol{x}\right)$, is not adequate when $s\neq 0$. The correct prescription is to include the spin degrees of freedom and consider the Hamiltonian operator in the Hilbert space $\mathscr{H}_S=\mathscr{H}\otimes V_s$. For the case of an electron – particle with spin $\frac{1}{2}$ - the corresponding Hamiltonian is given by

$$H=\frac{1}{2m}\left(\boldsymbol{P}_A\cdot\boldsymbol{\sigma}\right)^2+e\varphi(\boldsymbol{x}),\quad \boldsymbol{P}_A=\boldsymbol{P}-\frac{e}{c}\boldsymbol{A}. \tag{2.2}$$

Using the basic facts that Pauli matrices anti-commute and satisfy $\sigma_1^2=\sigma_2^2=\sigma_3^2=I_2$ and

$$\sigma_1\sigma_2=i\sigma_3,\quad \sigma_2\sigma_3=i\sigma_1,\quad \sigma_3\sigma_1=i\sigma_2$$

we readily obtain

$$\begin{aligned}\left(\boldsymbol{P}_A\cdot\boldsymbol{\sigma}\right)^2&=\left(P_1-\frac{e}{c}A_1\right)^2+\left(P_2-\frac{e}{c}A_2\right)^2+\left(P_3-\frac{e}{c}A_3\right)^2\\&+i\left[P_1-\frac{e}{c}A_1,P_2-\frac{e}{c}A_2\right]\sigma_3+i\left[P_2-\frac{e}{c}A_2,P_3-\frac{e}{c}A_3\right]\sigma_1\\&+\quad+i\left[P_3-\frac{e}{c}A_3,P_1-\frac{e}{c}A_1\right]\sigma_2\\&=\left(\boldsymbol{P}-\frac{e}{c}\boldsymbol{A}\right)^2-\frac{\hbar e}{c}\left(B_1\sigma_1+B_2\sigma_2+B_3\sigma_3\right).\end{aligned}$$

Here $\boldsymbol{B}=(B_1,B_2,B_3)$ is the magnetic field, $\boldsymbol{B}=\operatorname{curl}\boldsymbol{A}$, and in the last line we have used Heisenberg commutation relations (cf. a similar computation in Example 2.3 in Section 2.4 of Chapter 2). The Hamiltonian (2.2) takes the form

$$H=H^0-\mu\boldsymbol{B}\cdot\boldsymbol{\sigma},\quad \mu=\frac{\hbar e}{2mc}, \tag{2.3}$$

and is known as the Pauli Hamiltonian; the quantity μ is the total magnetic moment of an electron. It is customary to put $\mu=-\mu_{\mathrm{B}}$, where

$$\mu_{\mathrm{B}}=\frac{\hbar|e|}{2mc}=0.927\times10^{-20}\frac{\mathrm{erg}}{\mathrm{gauss}}$$

is the so-called Bohr magneton. The corresponding time-dependent Schrdinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi$$

in this context is called the Pauli wave equation.

Remark. The Pauli wave equation is obtained from the relativistic Dirac equation for the electron in the limit $c \to \infty$ by neglecting the terms of order c^{-2}.

The corresponding Hamiltonian for a quantum particle of spin s and charge e has a similar form

$$H = H^0 - \boldsymbol{B}\cdot\boldsymbol{\mu}, \quad \boldsymbol{\mu} = \frac{\mu}{\hbar s}\boldsymbol{S},$$

where $S = (S_1, S_2, S_3)$ are spin operators of spin s, quantity μ is the total magnetic moment of a particle, and the operator $\boldsymbol{\mu}$ is its "intrinsic" magnetic moment.

10.1.5 2.2. Particle in a uniform magnetic field by Tahtajan

Here we consider the problem of finding the energy levels of a charged spin $\frac{1}{2}$ particle moving in a constant uniform magnetic field. Choosing the z-axis along the direction of the field, $\boldsymbol{B} = (0, 0, B)$, we get $A_1(\boldsymbol{x}) = -By, A_2(\boldsymbol{x}) = A_3(\boldsymbol{x}) = 0$, and $\varphi(\boldsymbol{x}) = 0$. The Pauli Hamiltonian takes the form

$$H = \frac{1}{2m}\left[\left(P_1 + \frac{e}{c}By\right)^2 + P_2^2 + P_3^2\right] - \mu B\sigma_3 \tag{2.4}$$

The eigenvalue equation

$$H\psi(\boldsymbol{x},\sigma) = E\psi(\boldsymbol{x},\sigma)$$

in $\mathscr{H}_S$ reduces to two (for each value of $\sigma = \pm\frac{1}{2}$) eigenvalue equations

$$\frac{1}{2m}\left[\left(P_1 + \frac{e}{c}By\right)^2 + P_2^2 + P_3^2\right]\psi - \mu B\sigma\psi = E\psi$$

in $\mathscr{H}$. Separating the variables

$$\psi(\boldsymbol{x}) = e^{\frac{i}{\hbar}(k_1x + k_3z)}\chi(y)$$

we obtain

$$-\frac{\hbar^2}{2m}\chi'' + \frac{m\omega_{\mathrm{B}}^2}{2}(y - y_0)^2\chi = \left(E + \mu B\sigma - \frac{k_3^2}{2m}\right)\chi \tag{2.5}$$

where

$$y_0 = -\frac{ck_1}{eB} \quad \text{and} \quad \omega_{\mathrm{B}} = \frac{|e|B}{mc}$$

Equation (2.5) coincides with the eigenvalue problem for the one-dimensional harmonic oscillator with the frequency ω_{B}, solved in Section 2.6 of Chapter 2. Thus we obtain

$$E = \left(n + \frac{1}{2}\right)\hbar\omega_{\mathrm{B}} + \frac{k_3^2}{2m} - \mu B\sigma, \quad n = 0, 1, ...; \quad \sigma = \pm\frac{1}{2} \tag{2.6}$$

The first term in this formula gives discrete energy levels, called Landau levels, for the motion in the plane perpendicular to the magnetic field.

The spectrum of Pauli Hamiltonian (2.4) is absolutely continuous and fills $\left[\frac{1}{2}\left(\hbar\omega_{\mathrm{B}}-\mu B\right),\infty\right)$ with variable infinite multiplicity. It can be visualized as a countable union of branches $\left[\left(n+\frac{1}{2}\right)\hbar\omega_{\mathrm{B}}-\mu B\sigma,\infty\right)$, each with a multiplicity parametrized by $\mathbb{R}\times\{\pm 1\}$ (all $k_1\in\mathbb{R}$ and $\pm k_3$ for fixed k_3
correspond to the same E). Corresponding normalized eigenfunctions of the continuous spectrum are
$\psi_n\left(\boldsymbol{x};k_1,k_3\right)=\frac{1}{2\pi\hbar}\sqrt[4]{\frac{m\omega_{\mathrm{B}}}{\pi\hbar}}\frac{1}{\sqrt{2^n n!}}e^{\frac{i}{\hbar}(k_1x+k_3z)-\frac{m\omega_{\mathrm{B}}}{2\hbar}(y-y_0)^2}H_n\left(\sqrt{\frac{m\omega_{\mathrm{B}}}{\hbar}}y\right)$,
where $-\infty<k_1,k_3<\infty$.
For the electron, $\hbar\omega_{\mathrm{B}}=\frac{1}{2}\mu_{\mathrm{B}}$, and formula (2.6) takes the form

$$E=\left(n+\frac{1}{2}+\sigma\right)\mu_{\mathrm{B}}B+\frac{k_3^2}{2m}.$$

In this case there is an extra degeneration of the spectrum: energy levels with n and $\sigma=\frac{1}{2}$ and those with $n+1$ and $\sigma=-\frac{1}{2}$ coincide.
Problem 2.1. Derive the eigenfunction expansion theorem for the Hamiltonian (2.4).

Problem 2.2. Show that the operators

$$X_0=Q_1+\frac{c}{eB}P_2\quad\text{ and }\quad Y_0=-\frac{c}{eB}P_1,$$

which correspond to the coordinates of a center of a circle (see Problem 1.5 in Section 1.3 of Chapter 1), are quantum integrals of motion, i.e., commute with the Hamiltonian H, but

$$\{X_0,Y_0\}_\hbar=\frac{c}{eB}I.$$

10.1.6 Motion in magnetic field in Dirac notation

(тут другое решение этой задачи)

Model of Dirac particle in a monolayer of graphene in magnetic field

(тут неплохо бы вставить теоирю про графен, что так-то можно разделить его на две подрешетки K, K', найти дисперс. соотношение. Про это отдельно нужно думать и это не тема этого раздела. потом коротко напишу то, что нужно для задачи ниже из этого.)

The low-energy properties, corresponding to the electronic states near the Fermi energy, can be described by expanding the energy dispersion around the K and K′ points. Let us write the graphene wave vector for valley K as $\mathbf{q}=\mathbf{K}+\mathbf{k}$. What we get for $|\mathbf{k}|\ll 1$ is

$$\epsilon(\mathbf{K}+\mathbf{k})\approx\pm\hbar v_F|\mathbf{k}|$$

where $v_F=\frac{3a|t|}{2\hbar}\approx 10^6$ m/s is Fermi velocity (which is comparable to that in metals). The expression for the expansion around K' is the same. The expression (3) corresponds to the two cones meeting at the K point with linear dependence on the wave vector. Because we know, that energy dispersion which is linear in wave vector belongs to massless particles, we say that electrons and holes with wave vectors close to K and K' points behave as massless. Those massless Dirac fermions made study of monolayer graphene so enticing.

As we know from particle physics, (almost) massless neutrinos are not described by Schrödinger equation, but by Dirac equation. Therefore, we would like to see whether Hamiltonian ascribed to our system (1) also have the form of Hamiltonian in the Dirac

equation. Since particles behave as massless only around the K and K', we expand the Hamiltonian

$$H(\mathbf{q}) = \begin{pmatrix} \epsilon_0 & tg(\mathbf{q}) \\ tg(\mathbf{q})^* & \epsilon_0 \end{pmatrix}$$

around these points as well. The Hamiltonian in the vicinity of the K point is for $\mathbf{q} = \mathbf{K}+\mathbf{k}$

$$H_K^0(\mathbf{k}) = \hbar v_F \begin{pmatrix} 0 & i\left(k_x - ik_y\right) \\ -i\left(k_x + ik_y\right) & 0 \end{pmatrix}$$

which does not yet fully resemble the form of Dirac equation. To get rid of the imaginary factors, which spoil the equivalence, we redefine wavefunctions containing coefficients $c_{\alpha,\beta}$ as

$$\Psi_0^K = \begin{pmatrix} c_{A,K} \\ c_{B,K} \end{pmatrix} \rightarrow \Psi^K = \begin{pmatrix} -ic_{A,K} \\ c_{B,K} \end{pmatrix}, \quad \Psi_0^{K'} = \begin{pmatrix} c_{A,K'} \\ c_{B,K'} \end{pmatrix} \rightarrow \Psi^{K'} = \begin{pmatrix} c_{A,K'} \\ -ic_{B,K'} \end{pmatrix}$$

and consequently change the Hamiltonian, so that equations, coming from each line of the matrix representation of $H_K\Psi_K = \epsilon\Psi_K$, do not change. The new Hamiltonian is then

$$H_K(\mathbf{k}) = \hbar v_F \vec{\sigma} \cdot \mathbf{k}$$

where the $\vec{\sigma} = (\sigma_x, \sigma_y)$ is a vector of Pauli matrices. For the Hamiltonian in the vicinity of the K' holds $H_{K'}(\mathbf{k}) = -H_K^T(\mathbf{k})$. In relation with Dirac equation, we call the wavefunction Ψ^β spinor. In its upper and lower term it has the quantum mechanical amplitudes of finding the particle in one of the two sublattices A and B, respectively. And for each valley K and K' we have one such spinor. If we put them together in one bispinor $\Psi = \left(\Psi^{K'}, \Psi^K\right)^T$ and both Hamiltonian in a common one, we get

$$H\Psi = v_F \begin{pmatrix} -\vec{\sigma}^* \cdot \mathbf{p} & 0 \\ 0 & \vec{\sigma} \cdot \mathbf{p} \end{pmatrix} \Psi$$

Although we speak of Dirac particles, equation (6) is not completely the same as true Dirac equation which would be in chiral representation equal to

$$H\Psi = c \begin{pmatrix} -\vec{\sigma} \cdot \mathbf{p} & 0 \\ 0 & \vec{\sigma} \cdot \mathbf{p} \end{pmatrix} \Psi$$

The motion of relativistic charges in graphene in a strong magnetic field is also quantized. In a conventional electron gas (non-relativistic) Landau quantization produces equidistant energy levels, which is due to the parabolic dispersion law of free electrons. In graphene the electrons have relativistic dispersion law, which strongly modifies the Landau quantization of the energy and the position of the levels.

As for free electrons, we make the substitution $p_i \rightarrow p_{0i} = p_i - \frac{e}{c}A_i$. The Hamiltonian (6) will therefore change to

$$H = v_F \begin{pmatrix} 0 & -\left(p_{0x} + ip_{0y}\right) & 0 & 0 \\ -\left(p_{0x} - ip_{0y}\right) & 0 & 0 & 0 \\ 0 & 0 & 0 & p_{0x} - ip_{0y} \\ 0 & 0 & p_{0x} + ip_{0y} & 0 \end{pmatrix}$$

where the four-component wave function

$$\Psi = \begin{pmatrix} \Phi_A^{K'} \\ \Phi_B^{K'} \\ \Phi_A^K \\ \Phi_B^K \end{pmatrix}$$

corresponding to the Hamiltonian (9) now takes on broader meaning, such that Φ_A^K and Φ_B^K are envelope wavefunctions of A and B sites for the valley K, and $\Phi_A^{K'}, \Phi_B^{K'}$ for the valley K '.

For the magnetic field orthogonal to the graphene layer, the vector potential can be chosen in Landau gauge as $A = (-By, 0)$. For such gauge, $[H, \hat{p}_x] = 0, p_x$ is good quantum number. Because equations for K and K′ valley are decoupled, let us first look for the solutions of the K valley. We are solving the system

$$\begin{aligned}\epsilon\Phi_A^K &= v_F\left(\hat{p}_{0x} - i\hat{p}_{0y}\right)\Phi_B^K \\ \epsilon\Phi_B^K &= v_F\left(\hat{p}_{0x} + i\hat{p}_{0y}\right)\Phi_A^K\end{aligned}$$

which can be by inserting one equation into another further decoupled into

$$\begin{aligned}\epsilon^2\Phi_A^K &= v_F^2\left(p_{0x} - ip_{0y}\right)\left(p_{0x} + ip_{0y}\right)\Phi_A^K \\ \epsilon^2\Phi_B^K &= v_F^2\left(p_{0x} + ip_{0y}\right)\left(p_{0x} - ip_{0y}\right)\Phi_B^K\end{aligned}$$

Let us find the energy levels ϵ for the Φ_B^K, using $[H, \hat{p}_x] = 0$ and that for electron $e = -e_0$

$$\begin{aligned}\frac{\epsilon^2}{v_F^2}\Phi_B^K &= \left(\left(\hat{p}_x + \frac{e}{c}B\hat{y}\right) + i\hat{p}_y\right)\left(\left(\hat{p}_x + \frac{e}{c}B\hat{y}\right) - i\hat{p}_y\right)\Phi_B^K \\ &= \left(\left(\hat{p}_x + \frac{eB}{c}\hat{y}\right)^2 - i\left[\hat{p}_x + \frac{eB}{c}\hat{y}, \hat{p}_y\right] + \hat{p}_y^2\right)\Phi_B^K \\ &= \left(\left(p_x + \frac{eB}{c}\hat{y}\right)^2 + \frac{\hbar eB}{c} + \hat{p}_y^2\right)\Phi_B^K \\ \frac{1}{2m}\left(\frac{\epsilon^2}{v_F^2} + \frac{\hbar e_0 B}{c}\right)\Phi_B^K &= \left(\frac{\tilde{k}}{2}\left(\hat{y} - y_0\right)^2 + \frac{\hat{p}_y^2}{2m}\right)\Phi_B^K\end{aligned}$$

Where $\tilde{k} = \frac{e_0 B}{c\sqrt{m}}, y_0 = \frac{p_x c}{e_0 B}$. Again the right side of the equation has the form of Hamiltonian for the harmonic oscillator, oscillating around y_0. If Φ_B^K is eigenfunction of such Hamiltonian, its eigenvalues will be $\hbar\omega_c\left(n + \frac{1}{2}\right)$ where as for the standard Landau quantization $\omega_c = \sqrt{\frac{k}{m}} = \frac{c_0 B}{mc}$. Consequently, the energy values for Landau levels in graphene monolayer must satisfy

$$\frac{\epsilon^2}{v_F^2} = \frac{\hbar e_0 B}{c}(2n + 1 - 1)$$

where $n = 0, 1, 2...$ goes through the same values as for harmonic oscillator. Since ϵ has positive and negative roots, we can extend the domain of n to integer values and write energy levels as

$$\epsilon = \mathrm{sgn}(n)\sqrt{\frac{2\hbar e_0 B}{c}}v_F\sqrt{|n|} = \hbar\omega^{\mathrm{Dirac}}\ \mathrm{sgn}(n)\sqrt{|n|}, \quad \omega^{\mathrm{Dirac}} = v_F\sqrt{\frac{2e_0 B}{\hbar c}}$$

The Landau level index, n, can be positive or negative. The positive values correspond to electrons (conduction band), while the negative values correspond to holes (valence band). Furthermore, they are not equidistant as in conventional case and the largest energy separation is between the zero and the first Landau level. This large gap allows one to observe the quantum Hall effect in graphene, even at room temperature (Physical Review B, 65(24):245420, 2002.).

In the above derivation we disregarded the spin of the electron, which brings additional twofold degeneracy of the Landau levels due to the spin. Because we are working with electrons in magnetic field, this degeneracy is actually splitted by the Zeeman interaction. Having derived the energy difference between successive Landau levels, we can compare it to the strength of

Zeeman interaction. For $B = 10T$, ratio between the latter and the difference between n = 1, 0 Landau level is

$$\frac{\hbar\omega_c/2}{v_F\sqrt{e\hbar B/c}} \approx 0.01$$

which in a way justifies our assumption for spin degeneration. If we repeat the whole procedure also for equation (10) with Φ_A^K, we get

$$\frac{\epsilon^2}{v_F^2} = \frac{\hbar e_0 B}{c} 2(n+1), \quad n = 0, 1, ...$$

which, comparing to the previous result for Φ_B^K, lacks the level with $\epsilon = 0$. In terms of the occupation of the sublattices A and B, we can therefore expect interesting properties. Specifically, the wave function at the Landau level $n \neq 0$ should always have non-zero amplitudes on both sublattices A and B, while the wavefunctions at the Landau level $n = 0$ should have non-zero amplitude only on one sublattice: B sublattice for valley K or A sublattice for valley K '. The asymmetry between A and B sublattice originates from asymmetry in positions of the nearest neighbors for atoms at A and B sublattice. This property of the wavefunctions for the Landau levels in graphene makes the $n = 0$ level very special for different magnetic applications of graphene.

The wave functions corresponding to the Landau levels (13) are labeled by three indices (nLandau level index, k -wave vector along the x -axis, K, K '-valley of wave vectors) and are given by the following expressions (Physical Review B, 65(24):245420, 2002.)

$$\Psi_{n,k}^K = \frac{C_n}{\sqrt{L}} e^{-ikx} \begin{pmatrix} 0 \\ 0 \\ \mathrm{sgn}(n)(-i)\phi_{|n|-1,k} \\ \phi_{|n|,k} \end{pmatrix}$$

for valley K and

$$\Psi_{n,k}^{K'} = \frac{C_n}{\sqrt{L}} e^{-ikx} \begin{pmatrix} \phi_{|n|,k} \\ \mathrm{sgn}(n)(-i)\phi_{|n|-1,k} \\ 0 \\ 0 \end{pmatrix}$$

for valley K . Here L^2 is the area of the system,

$$C_n(x) = \begin{cases} 1 & \text{for n} = 0, \\ \frac{1}{\sqrt{2}} & \text{for } n \neq 0 \end{cases}, \quad \mathrm{sgn}(n) = \begin{cases} 0 & \text{for n} = 0, \\ \frac{n}{|n|} & \text{for } n \neq 0 \end{cases}$$

$$\phi_{n,k} \propto \exp\left(-\frac{1}{2}\frac{(y - kl_B^2)^2}{l_B^2}\right) H_n\left[\frac{(y - kl_B^2)}{l_B}\right]$$

where $l_B = \sqrt{\hbar/eB}$ is the magnetic length and $H_n(x)$ are Hermite polynomials. $\phi_{n,k}$ is the wavefunction for a non-relativistic electron at the nth Landau level. All in all, their structure is reasonable: they are obviously eigenfunction of $\hat{p_x}$, in the $n = 0$ level only one sublattice is occupied and $(-i)$ factor comes from the redefinition of coefficients c_α. Another consequence of different dependence of energy levels on index n $\left(\epsilon_A \propto \sqrt{|n|-1}, \epsilon_B \propto \sqrt{|n|}\right)$ for sublattices A and B results also in different wavefunctions $\phi_{n,k}$ at both sites, which must differ in their index n for 1 to yield the same energy eigenvalue for both. Figure 3 shows the the profile of wavefunctions in the K valley along the y -axis for the sublattices A and B in magnetic field B = 10 T for the index n = 3.

Model of Dirac particle in a mbilayer of graphene in magnetic field

When two graphene layers stack to form a bilayer, the interlayer coupling leads to the appearance of band mass but it does not open a gap at the Dirac points. Here the Landau level spectrum takes the form

$$E_n = \mathrm{sgn}(n)\hbar\omega_c\sqrt{|n|(|n|-1)}, \quad n \in Z, \quad \omega_c = \frac{eB}{m^*c}$$

This sequence is linear in field, similar to the standard case, but it contains an additional zero-energy level, which is independent of the field.

(я удивлен, что такое решение только в одной методичке находится. в статьях что-то сложнее и эксперименты, но конкретно этого вывода я не находил.)

Details of model of Dirac particle in graphene in magnetic field

Почему все-таки формулы отличны от тех, которые для обычной частицы и как из одних перейти в другие?

(ведь эти модели связаны. приведу переход от одной модели к другой. пока не думал про это еще.)

Experimental differences of these models

(это упомянуто в начале статьи Magnetic oscillations in planar systems with the Dirac-like spectrum of quasiparticle excitations II: transport properties by V.P. Gusynin and S.G. Sharapov, пока не до этого)

Experimental confirmation of LL levels in graphene

(тонна статей про это, какую вставить - пока не знаю, потом прочитаю пару, вставлю самые полезные и разные графики типичные, разбираться в них еще нужно.)

On Landau Level Splitting in Graphene in High Magnetic Fields by Y. Zhang et. al.

(известаная статья что эксп. подтвердили, потом почитаю)
In summary, they report the observation of splittings of LLs in high quality graphene samples under high magnetic field up to 45 T. They discover the $n = 0$LL splits into four sublevels, lifting spin and sublattice degeneracy, potentially indicating a many-body correlation in this LL. In the $n = \pm 1$LL, only the spin degeneracy seems to be lifted within experimentally accessible high magnetic field. The effective g-factors were found close to the bare electron g-factor.

Link of LL levels and Quantum Hall effect

(тоже куча статей про это есть, уже в записи по КЭХ это написано, додумаю - и напишу сюда тоже)

Explanation from Two-Dimensional Gas of Massless Dirac Fermions in Graphene by K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, M.I. Katsnelson, I.V. Grigorieva, S.V. Dubonos, A.A. Firsov

To explain the half-integer QHE qualitatively, we invoke the formal expression [9-12] for the energy of massless relativistic fermions in quantized fields, $E_N = [2e\hbar {c_*}^2 B(N + 1/2 \pm 1/2)]^{1/2}$. In QED, sign $\pm$ describes two spins whereas in the case of graphene it refers to "pseudospins". The latter have nothing to do with the real spin but are "built in" the Dirac-like spectrum of graphene, and their origin can be traced to the presence of two carbon sublattices. The above formula shows that the lowest LL($N = 0$) appears at $E = 0$ (in agreement with the index theorem) and accommodates fermions with only one (minus) projection of the pseudospin. All other levels $N \geq 1$ are occupied by fermions with both ($\pm$) pseudospins. This implies that for $N = 0$ the degeneracy is half of that for any other N. Alternatively, one can say that all LL have the same "compound" degeneracy but zeroenergy LL is shared equally by electrons and holes. As a result the first Hall plateau occurs at half the normal filling and, oddly, both $v = -1/2$ and $+1/2$ correspond to the same LL ($N = 0$). All other levels have normal degeneracy $4B/\phi_0$ and, therefore, remain shifted by the same $1/2$ from the standard sequence. This explains the QHE at $v = N + 1/2$ and, at the same time, the "odd" phase of SdHO (minima in ρ_{xx} correspond to plateaux in ρ_{xy} and, hence, occur at half-integer v; see Figs. 2&3), in agreement with theory [9-12]. Note however that from another perspective the phase shift can be viewed as the direct manifestation of Berry's phase acquired by Dirac fermions moving in magnetic field [15, 16].

10.2 Selection Rules

Правила отбора по Нохриной

Рассмотрим в качестве примера применения теоремы Вигнера-Эккарта правила отбора для дипольного излучения в атомах. Плотность вероятности перехода из начального состояние в конечное с дипольным излучением пропорциональна следующему матричному элементу оператора проекции дипольного момента $\hat{d}_i$ (см., например, |1|) : $dw_{fi} \propto \left\langle J'M' \left| \hat{d}_i \right| JM \right\rangle$. Соответственно, "Запрещены" те переходы, для которых эти матричные элементы равны нулю. Анализ того, какие матричные элементы могут иметь нетривиальное значение, и приводит к правилам отбора для дипольного излучения.

Пример 8. Правила отбора по J. В качестве сферического тензора $\hat{T}_q^{(k)}$ рассмотрим набор операторов из примера 5. В этом случае $k = 1, q = -1, 0, 1$:

$$\hat{B}_0^{(1)} = \hat{d}_z, \quad \hat{B}_{\pm 1}^{(1)} = \mp \frac{1}{\sqrt{2}} \hat{d}_{\pm}.$$

Матричные элементы для компонент сферического тензора $\hat{B}_q^{(1)}$ в соответствии с утверждением теоремы Вигнера-Эккарта записываются в виде

$$\left\langle J'M' \left| \hat{d}_z \right| JM \right\rangle = \Lambda_0 (J, J') K_{J,M,1,0}^{J',M'},$$
$$\frac{\mp 1}{\sqrt{2}} \left\langle J'M' \left| \hat{d}_{\pm} \right| JM \right\rangle = \Lambda_{\pm} (J, J') K_{J,M,1,\pm 1}^{J',M'},$$

где коэффициенты пропорциональности Λ_0 и $\Lambda_{\pm}$зависят только от чисел J и J', и мы восстановили все индексы в записи коэффициентов Клебша-Гордана. Коэффициенты Клебша-Гордана в правых частях равенств могут быть не равны нулю, только если квантовые числа суммарного момента принимают допустимый диапазон значений. В нашем случае J' - это допустимые квантовые числа, характеризующие квадрат

суммарного момента, при сложении моментов J и 1. Из техники сложения моментов сле-13 дует, что

$$J' = \begin{cases} J+1 \\ J \\ J-1 \end{cases}$$

Значит, ненулевыми матричными элементами для операторов $\hat{d}_i$ могут быть только матричные элементы с квантовыми числами J и J', удовлетворяющими первому правилу отбора:

$$|J' - J| \leq 1$$

Пример 9. При сложении моментов, характеризуемых орбитальными квантовыми числами J и 1, имеем: при $J = 0$ суммарный момент $J' = 1$, при $J = 1$ суммарный момент $J' = \{0, 1, 2\}$ и так далее. То есть при $k = 1$ равенство $J = J' = 0$ не может быть выполнено. Значит, соответствующий коэффициент Клебша-Гордана, а вместе с ним и матричный элемент для операторов $\hat{d}_i$ равны нулю. Отсюда второе правило отбора:

$$\text{переход } J = 0 \to J' = 0 \text{ запрещен.}$$

Пример 10. Правило отбора для проекции момента следует из сложения моментов:

$$M' = M + 0 \quad \text{или} \quad M' = M \pm 1.$$

Все коэффициенты Клебша-Гордана для других M и M' равны нулю, отсюда следует третье правило отбора по проекции суммарного момента:

$$|M' - M| \leq 1$$

У пражнение. Получите правила отбора для состояний, описываемых квантовыми числами $S, M_{\mathrm{S}}, L, M_{\mathrm{L}}$.

правила отбора по Киселеву

Коэффициенты Клебша-Гордана принимают ненулевые значения, только если моменты и их проекции при сложении пробегают допустимую область своего изменения.

Поэтому и матричные элементы неприводимых тензорных операторов, пропорциональные, как мы убедились согласно теореме Вигнера-Эккарта, коэффициентам Клебша-Гордана, отличны от нуля, если, Во-первых,

$$M' = M + m, \quad m \in \{-j, -j+1, ..., j-1, j\}$$

Значит для оператора ранга j с произвольной допустимой проекцией имеет место, как говорят, правило отбора по проекции момента

$$|\Delta M| \leqslant j$$

В противном случае, матричные элементы этого оператора заведомо равны нулю.

Во-вторых, так как

$$|J - j| \leqslant J' \leqslant J + j$$

правило отбора по модулю момента принимает вид

$$|\Delta J| \leqslant j, \quad j \leqslant J + J'$$

Как следствие, получаем правило запрета: если $j \neq 0$, то матричные элементы с $J = J' = 0$ тож дественно равны нулю, или, как говорят, переход $0 \to 0'$ запрещен.

Примеры применения правил отбора в квантовой теории излучения (!!!)

(очень важно указать, иначе невозможно будет ими пользоваться.)

как происходит поглощение атомом фотона?

(напишу потом)

Если фотон берется из флуктуации вакуума, то можно ли черпать из флуктуации вакуума бесконечно энергию (??)

(? остался вопрос, не знаю, почему нет?)

Фактор Ланде

(?? тут что ли его подробно и обсудим???)

При решении задачи об эффекте Зеемана в слабом поле возникает необходимость вычислять матричные элементы вида

$$\left\langle JM' \left| \hat{S}_z + \hat{J}_z \right| JM \right\rangle .$$

14 Решение этой задачи базируется на введении фактора Ланде. Для вычисления этого фактора докажем несколько вспомогательных утверждений.

Утверждение 11. Матричные элементы операторов $\hat{S}_i$ и $\hat{J}_i$ пропорциональны друг другу, а коэффициент пропорциональности зависит только от квантового числа J.

Доказательство. Операторы $\hat{S}_z$ и $\mp\hat{S}_\pm/\sqrt{2}$ являются компонентами сферического тензора $\hat{A}^{(1)}_q$ (см. Пример 1). Применим к ним теорему Вигнера-Эккарта:

$$\left\langle JM' \left| \hat{S}_z \right| JM \right\rangle = \Lambda_0(J) K^{J,M'}_{M,0} ,$$
$$\frac{\mp 1}{\sqrt{2}} \left\langle JM' \left| \hat{S}_\pm \right| JM \right\rangle = \Lambda_\pm(J) K^{J,M'}_{M,\pm 1}.$$

Применяя теорему к сферическому тензору, компонентами которого являются $\hat{J}_z$ и $\mp\frac{1}{\sqrt{2}}\hat{J}_\pm$, получим

$$\left\langle JM' \left| \hat{J}_z \right| JM \right\rangle = \widetilde{\Lambda}_0(J) K^{J,M'}_{M,0} ,$$
$$\frac{\mp 1}{\sqrt{2}} \left\langle JM' \left| \hat{J}_\pm \right| JM \right\rangle = \widetilde{\Lambda}_\pm(J) K^{J,M'}_{M,\pm 1}.$$

Сравнивая равенства (9) и (10), получаем, что матричные элементы операторов $\hat{S}_i$ и $\hat{J}_i$ пропорциональны друг другу:

$$\left\langle JM' \left| \hat{S}_z \right| JM \right\rangle = \frac{\widetilde{\Lambda}_0(J)}{\Lambda_0(J)} \left\langle JM' \left| \hat{J}_z \right| JM \right\rangle ,$$
$$\left\langle JM' \left| \hat{S}_x \right| JM \right\rangle = \frac{\widetilde{\Lambda}_+(J) + \widetilde{\Lambda}_-(J)}{\Lambda_+(J) + \Lambda_-(J)} \left\langle JM' \left| \hat{J}_x \right| JM \right\rangle ,$$
$$\left\langle JM' \left| \hat{S}_y \right| JM \right\rangle = \frac{\widetilde{\Lambda}_+(J) - \widetilde{\Lambda}_-(J)}{\Lambda_+(J) - \Lambda_-(J)} \left\langle JM' \left| \hat{J}_y \right| JM \right\rangle .$$

Утверждение 12. Коэффициенты пропорциональности в равенствах (11) - (13) равны, и, значит, выполнено

$$\left\langle JM' \left| \hat{S}_i \right| JM \right\rangle = \Lambda(J) \left\langle JM' \left| \hat{J}_i \right| JM \right\rangle ,$$

где коэффициент $\Lambda(J)$ не зависит от i.

Доказательство. Вспомним, что векторы $\varphi_{LM_L}, \psi_{SM_S}$ и операторы $\hat{L}_i, \hat{S}_i$ могут быть записаны в представлении, собств енном для операторов $\hat{L}^2, \hat{L}_z$ и $\hat{S}^2, \hat{S}_z$ соответственно, где подразумевается, что в координатном пространстве $\mathbb{R}^3$ выбрана система координат K с осями OX, OY и OZ. То есть выбрано представление, собственное для проекции момента и спина на ось OZ. То же самое в ерно для в екторов Ψ_{JM} и операторов $\hat{J}_i$.

Поворотом преобразуем систему координат K в систему K' так, чтобы ось OX совпадала с осью OZ'.С одной стороны, в системе K' векторы, записанные в представлении, собств енном для проекции спина и момента на ось OZ', будут иметь те же компоненты, что и векторы, записанные в представлении, собственном для проекции спина или момента на ось OZ в системе K. Например, вектор проекции спина на ось OZ', равной $+\hbar/2$, в собственном представлении записывается в виде

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Будем обозначать в се векторы и операторы, записанные в представлении, собств енн ом для проекции момента на ось OZ', штрихом. Тогда выполнено равенство

$$\left(\Psi'_{JM'}, \hat{S}'_z \Psi'_{JM}\right) = \left(\Psi_{JM'}, \hat{S}_z \Psi_{JM}\right)$$

Таким образом,

$$\left(\Psi'_{JM'}, \hat{S}'_z \Psi'_{JM}\right) = \frac{\tilde{\Lambda}_0(J)}{\Lambda_0(J)} \left(\Psi_{JM'}, \hat{J}_z \Psi_{JM}\right)$$

С другой стороны, переход из OZ - представдения в OZ' - представление может быть осуществлен повором осей. Такое преобразование реализуется унитарными матрицами [1]:

$$\varphi'_{SM_S} = U_S \varphi_{SM_S},$$
$$\psi'_{LM_L} = U_L \psi_{LM_L}$$

16 Соответственно,

$$\Psi'_{JM} = \sum K^{J,M}_{S,M_S,L,M_L} \varphi'_{SM_S} \otimes \psi'_{LM_L} =$$
$$= \sum K^{J,M}_{S,M_S,L,M_L} \left(U_S \otimes U_L\right) \varphi_{SM_S} \otimes \psi_{LM_L} =$$
$$= \left(U_S \otimes U_L\right) \Psi_{JM} = U \Psi_{JM},$$

где $U = U_S \otimes U_L$ унитарна. Рассмотрим цепочку равенств

$$\left(\Psi_{JM'}, \hat{S}_x \Psi_{JM}\right) = \left(\Psi_{JM'}, U^{-1} U \hat{S}_x U^{-1} U \Psi_{JM}\right) =$$
$$= \left(U \Psi_{JM'}, \left(U \hat{S}_x U^{-1}\right) U \Psi_{JM}\right) = \left(\Psi'_{JM'}, \hat{S}'_z \Psi'_{JM}\right).$$

Таким образом, мы получили, что

$$\left(\Psi_{JM'}, \hat{S}_x \Psi_{JM}\right) = \left(\Psi'_{JM'}, \hat{S}'_z \Psi'_{JM}\right) =$$
$$= \frac{\tilde{\Lambda}_+(J) + \tilde{\Lambda}_-(J)}{\Lambda_+(J) + \Lambda_-(J)} \left(\Psi_{JM'}, \hat{J}_z \Psi_{JM}\right).$$

Из равенств (14) - (15) следует, что

$$\frac{\tilde{\Lambda}_0(J)}{\Lambda_0(J)} = \frac{\tilde{\Lambda}_+(J) + \tilde{\Lambda}_-(J)}{\Lambda_+(J) + \Lambda_-(J)}.$$

Будем обозначать каждое из отношений в этом равенстве $\Lambda(J)$. Аналогично доказываются и остальные равенства.

Вспомним задачу о сложении моментов и освежим в памяти обознач ения [4]. Пусть складываются моменты L и S. Это значит, что мы работаем в пространстве $\mathcal{M} = \mathbb{C}^{(2S+1)} \otimes \mathbb{C}^{(2L+1)}$. В процессе сложения моментов мы строим изометрический изоморфизм

$$\mathcal{M} \cong \bigoplus_{K=|L-S|}^{L+S} \mathbb{J}_K$$

где $\mathbb{J}_K$ - собственные для оператора $\hat{J}^2$ подпространства. Мы строим операторы суммарного момента так, чтобы матричные элементы вне $\mathbb{J}_K$ были равны нулю:

$$\left\langle JM \left| \hat{J}_i \right| J'M' \right\rangle \propto \delta_{JJ'} \quad \text{и} \quad \left\langle JM \left| \hat{J}^2 \right| J'M' \right\rangle \propto \delta_{JJ'}$$

Ниже нам понадобится работать с операторами, суженными на некоторое подпростр анство (причём на подпространство, необязательно собственное для рассматриваемого оператора, - и в этом вся тонкость). Будем обозначать оператор $\hat{A}$, суженный на подпростр анство $\mathcal{N}$, так: $(\hat{A}|\mathcal{N})$. твержение 13. Операторы $\hat{1} \otimes \hat{S}_i$ и $\hat{L}_j \otimes \hat{1}$ в собственном для $\hat{J}^2$ и $\hat{J}_z$ представлении обязательно имеют ненулевые матричные элементы вне $\mathbb{J}_K$. Доказательство. А. Докажем, что $\hat{1} \otimes \hat{S}_z$ имеет ненулевые недиагональные элементы. Доказательства для остальных компонент и для всех компонент $\hat{\mathbf{L}} \otimes \hat{1}$ легко проводятся в собственном для соответствующей компоненты представлении и здесь не приведены, чтобы избежать загромождения. Итак, рассмотрим старший вектор $|J, J\rangle \cong |L, L\rangle \otimes |S, S\rangle$. Дейст уя на него оператором понижения и нор мируя, получи м в ектор

$$|J, J-1\rangle \cong \sqrt{\frac{L}{L+S}}|L, L-1\rangle \otimes |S, S\rangle + \sqrt{\frac{S}{L+S}}|L, L\rangle \otimes |S, S-1\rangle.$$

Этот вектор не является собственным для операторов $\hat{1} \otimes \hat{S}_z$ и $\hat{L}_z \otimes \hat{1}$. Значит, он может быть разложен на сумму в екторов $\Psi_{J,J-1}$ и ортогонального ему вектора $\beta \in \mathcal{M}$:

$$\hat{S}_z|J, J-1\rangle = \text{ const } \cdot |J, J-1\rangle + |\beta\rangle, \quad \text{где} \quad \langle J, J-1|\beta\rangle = 0.$$

Так как $(2L+1)(2S+1)$ векторов $|J, M\rangle$ образуют базис в $\mathcal{M}$, то существ ует вектор $|J', M'\rangle$, на который проекция $|\beta\rangle$ ненулевая. Это и доказывает наличие ненулевых недиагональных элементов оператора $\hat{1} \otimes \hat{S}_z$. Докажем теперь, что ненулевой недиагональный элемент может лежать лишь вне $\mathbb{J}_K$.

В. По определению $\hat{S}_z$ и $\hat{J}_z = \hat{L}_z \otimes \hat{1} + \hat{1} \otimes \hat{S}_z$ коммутируют на $\mathcal{M}$:

$$\left[\hat{S}_z, \hat{J}_z\right] = 0$$

Из этого следует, что

$$\left\langle J', M' \left| \left[\hat{S}_z, \hat{J}_z\right] \right| J, M \right\rangle = 0$$

$$M \cdot \left\langle J', M' \left| \hat{S}_z \right| J, M \right\rangle - M' \cdot \left\langle J', M' \left| \hat{S}_z \right| J, M \right\rangle = 0$$

Значит, матричный элемент $\left\langle J', M' \left| \hat{S}_z \right| J, M \right\rangle$ может быть не равен нулю только для $M = M'$. Так как матрица оператора $\hat{S}_z$ в выбранном представлении и меет ненулевые недиаг ональные элементы, а одинаковые кв антовые числа M и $M' = M$ могут принадлежать

только различным $\mathbb{J}_K$, то ненулевой недиагональный матричный элемент для $\hat{S}_z$ может лежать лишь вне собственных для $\hat{J}^2$ подпространств $\mathbb{J}_K$.

Пример 14. Рассмотрим сумму моментов $S = 1/2$ и $L = 1/2$ (формально L может принимать только целые значения, но наши рассуждения верны для суммы моментов любой природы, а обозначение L мы сохраним только для единообразия обозначений). J может принимать значения 1 и 0. Рутинные вычисления дают:

$$\hat{1} \otimes \hat{S}^2 = \frac{3}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\hat{1} \otimes \hat{S}_z = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

$$\hat{1} \otimes \hat{S}_x = \frac{1}{2\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ -1 & 0 & 1 & 0 \end{pmatrix}$$

$$\hat{1} \otimes \hat{S}_y = \frac{1}{2\sqrt{2}} \begin{pmatrix} 0 & i & 0 & -i \\ -i & 0 & i & 0 \\ 0 & -i & 0 & -i \\ i & 0 & i & 0 \end{pmatrix}$$

$$\hat{J}^2 = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \hat{J}_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\hat{J}_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \hat{J}_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Легко видеть, что операторы $\hat{1} \otimes \hat{S}_i$ имеют нетривиальные матричные элементы вне $\mathbb{J}_0$ и $\mathbb{J}_1$.

У твердждение 15. Если оператор $\hat{A}_i$ имеет только нулевые матричные элементы вне $\mathbb{J}_K$, то

$$\left(\hat{S}_i \hat{A}_i | \mathbb{J}_K\right) = \left(\hat{S}_i | \mathbb{J}_K\right) \left(\hat{A}_i | \mathbb{J}_K\right) = \left(\hat{S}_i | \mathbb{J}_K\right) \hat{A}_i$$

Здесь левая часть равенства означает, что сначала мы перемножаем матрицы операторов в выбранном представлении на $\mathcal{M}$, а потом сужаем результат на нужное подпространство, например, на $\mathbb{J}_K$. Средняя часть равенства означает, что сначала мы сужаем перемножаемые операторы на $\mathbb{J}_K$, а потом перемножаем матрицы меньшей размерности. Здесь также предполагается суммирование по повторяющемуся индексу.

Доказательство. Матричные элементы $\left(\hat{S}_i \hat{A}_i | \mathbb{J}_K\right)$ по опр еделению сужения равны

$$\left\langle J, M \left| \left(\hat{S}_i \hat{A}_i | \mathbb{J}_K\right) \right| J', M' \right\rangle = \left\langle K, M \left| \hat{S}_i \hat{A}_i \right| K, M' \right\rangle$$

Рассмотрим теперь матричные элементы произведения операторов на $\mathcal{M}\left(\hat{S}_i|\mathbb{J}_K\right)\hat{A}_i$:

$$\left\langle J,M\left|\left(\hat{S}_i|\mathbb{J}_K\right)\hat{A}_i\right|J',M'\right\rangle =$$
$$=\sum_{J'',M''}\left\langle J,M\left|\left(\hat{S}_i|\mathbb{J}_K\right)\right|J'',M''\right\rangle\left\langle J'',M''\left|\hat{A}_i\right|J',M'\right\rangle =$$
$$=\sum_{J'',M''}\left\langle K,M\left|\hat{S}_i\right|K,M''\right\rangle\delta_{J,K'}\delta_{K,J''}\left\langle J'',M''\left|\hat{A}_i\right|J',M'\right\rangle =$$
$$=\sum_{M''}\left\langle K,M\left|\hat{S}_i\right|K,M''\right\rangle\left\langle K,M''\left|\hat{A}_i\right|J',M'\right\rangle .$$

20 Так как матричные элементы $\hat{A}_i$ равны нулю вне $\mathbb{J}_K$, то

$$=\sum_{M''}\left\langle K,M\left|\hat{S}_i\right|K,M''\right\rangle\left\langle K,M''\left|\hat{A}_i\right|J',M'\right\rangle=\sum_{M''}\left\langle K,M\left|\hat{S}_i\right|K,M''\right\rangle\left\langle K,M''\left|\hat{A}_i\right|K,M'\right\rangle .$$

Так как на $\mathbb{J}_K$ множеств о $|K,M\rangle_{M=-K}^{M=K}$ является базисом, то последнее выражение равно

$$\sum_{M''}\left\langle K,M\left|\hat{S}_i\right|K,M''\right\rangle\left\langle K,M''\left|\hat{A}_i\right|K,M'\right\rangle =$$
$$=\left\langle K,M\left|\hat{S}_i\hat{A}_i\right|K,M'\right\rangle .$$

Отсюда получаем требуемое равенство:

$$\left\langle J,M\left|\left(\hat{S}_i|\mathbb{J}_K\right)\hat{A}_i\right|J',M'\right\rangle=\left\langle J,M\left|\left(\hat{S}_i\hat{A}_i|\mathbb{J}_K\right)\right|J',M'\right\rangle .$$

Замечание 16. В частности, для $\hat{A}_i=\hat{J}_i$ выполнено:

$$\left\langle J,M\left|\left(\hat{S}_i|\mathbb{J}_K\right)\hat{J}_i\right|J',M'\right\rangle=\left\langle J,M\left|\left(\hat{S}_i\hat{J}_i|\mathbb{J}_K\right)\right|J',M'\right\rangle .$$

Утверждение 17. Если оператор $\hat{A}_i$ имеет ненулевые элементы вне $\mathbb{J}_K$, то может быть

$$\left(\hat{S}_i\hat{A}_i|\mathbb{J}_K\right)\neq\left(\hat{S}_i|\mathbb{J}_K\right)\left(\hat{A}_i|\mathbb{J}_K\right)$$

Доказательство. В качестве доказательства приведем пример. Возьмем в качестве $\hat{A}_i$ операторы $\hat{S}_i$. Выберем $K=1$. Пользуясь матрицами из примера (14), пря мым вычислением получи м

$$\left\langle J,M\left|\left(\hat{S}_i\hat{S}_i|\mathbb{J}_1\right)\right|J',M'\right\rangle=\left\langle 1,M\left|\hat{S}_i\hat{S}_i\right|1,M'\right\rangle=\frac{3}{4}\delta_{M,M'}$$
$$\left\langle J,M\left|\left(\hat{S}_i|\mathbb{J}_1\right)\left(\hat{S}_i|\mathbb{J}_1\right)\right|J',M'\right\rangle =$$
$$=\sum_{J'',M''}\left\langle J,M\left|\left(\hat{S}_i|\mathbb{J}_1\right)\right|J'',M''\right\rangle\left\langle J'',M''\left|\left(\hat{S}_i|\mathbb{J}_1\right)\right|J',M'\right\rangle =$$
$$=\sum_{M''}\left\langle 1,M\left|\hat{S}_i\right|1,M''\right\rangle\left\langle 1,M''\left|\hat{S}_i\right|1,M'\right\rangle=\frac{1}{2}\delta_{M,M'}$$

21 Утверждение 18 (вычисление фактора Ланде). На каждом собственном для оператора $\hat{J}^2$ подпространстве выполнено

$$\left\langle JM'\left|\hat{S}_z+\hat{J}_z\right|JM\right\rangle=g_{LSJ}\left\langle JM'\left|\hat{J}_z\right|JM\right\rangle ,$$

где множитель

$$g_{LSJ} = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}$$

называется фактором Ланде. Доказательство. В соответствии с Утверждением 12 матричный элемент

$$\left\langle JM' \left| \hat{S}_z \right| JM \right\rangle = \Lambda(J) \left\langle JM' \left| \hat{J}_z \right| JM \right\rangle.$$

Для вычисления $\Lambda(J)$ запишем матричный элемент оператора

$$\left\langle JM' \left| \hat{S}_i \hat{J}_i \right| JM \right\rangle.$$

По определению на всем $\mathcal{M}$

$$\hat{\mathbf{S}} \cdot \hat{\mathbf{J}} = \hat{S}^2 - \frac{\hat{J}^2 - \hat{L}^2 - \hat{S}^2}{2}$$

Значит, матричный элемент (17) равен

$$\begin{aligned} &\left\langle JM' \left| \hat{S}^2 + \frac{1}{2}\left(\hat{J}^2 - \hat{L}^2 - \hat{S}^2\right) \right| JM \right\rangle = \\ =&\frac{J(J+1) - L(L+1) + S(S+1)}{2} \delta_{MM'} \end{aligned}$$

С другой стороны, в силу У тверждения 15 выполнено равенство

$$\begin{aligned} &\left\langle JM' \left| \hat{S}_i \hat{J}_i \right| JM \right\rangle = \\ &= \left\langle J'M' \left| \left(\hat{S}_i \hat{J}_i | \mathbb{J}_J \right) \right| \tilde{J}M \right\rangle = \\ = \sum_{J'',M''} &\left\langle J'M' \left| \left(\hat{S}_i | \mathbb{J}_J \right) \right| J''M'' \right\rangle \left\langle J''M'' \left| \left(\hat{J}_i | \mathbb{J}_J \right) \right| \tilde{J}M \right\rangle = \\ &= \sum_{M''} \left\langle JM' \left| \hat{S}_i \right| JM'' \right\rangle \left\langle JM'' \left| \hat{J}_i \right| JM \right\rangle. \end{aligned}$$

Матричные элементы $\left\langle JM' \left| \hat{S}_i \right| JM'' \right\rangle$ в силу Утверждения 12 могут быть записаны в виде

$$\left\langle JM' \left| \hat{S}_i \right| JM'' \right\rangle = \Lambda(J) \left\langle JM' \left| \hat{J}_i \right| JM'' \right\rangle.$$

Значит,

$$\begin{aligned} &\left\langle JM' \left| \hat{S}_i \hat{J}_i \right| JM \right\rangle = \\ = \Lambda(J) \sum_{M''} &\left\langle JM' \left| \hat{J}_i \right| JM'' \right\rangle \left\langle JM'' \left| \hat{J}_i \right| JM \right\rangle = \\ &= \Lambda(J) J(J+1) \delta_{MM'} \end{aligned}$$

Равенства (18) и (19) позволяют вычислять значение множителя $\Lambda(J)$ для каждого J:

$$\Lambda(J) = \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}.$$

Отсюда после простых вычислений следует искомое выражение (16) для фактора Ланде g_{LSJ}.

Обсуждение вывода фактора Ланде. Вычисление фактора Ланде опирается на вычисление матричных элементов оператора $\hat{1} \otimes \hat{S}_z$. Для этого в качестве технического приема рассматрив аются матричные элементы оператора $\hat{S}_i \hat{J}_i$. Исследование такого оператора позволяет вычислить фактор $\Lambda(J)$, пользуясь теоремой Вигнера-Эккарта. При этом именно Утверждения 15 и 17 позволяют провести вычисления, так как теорема Вигнера-Эккарта устанавливает пропорциональность матричных элементов сферических тензоров коэффициентам КлебшаГордана лишь на собственных для $\hat{J}^2$ подпространствах.

Для демонстрации важности аккуратного подхода к вычислению фактора Ланде хочется обратить внимание на следующий пример неверного вычисления g_{LSJ}. Из частного обсуждения с Алексеем Леонидовичем Барабановым: кажется, что можно вы-числять фактор Ланде следующим образом. Рассмотрим матричные элементы $\left\langle JM' | \hat{\mathbf{S}} \cdot \hat{\mathbf{S}} | JM \right\rangle$. С одной стороны, они равны

$$\left\langle JM' | \hat{\mathbf{S}} \cdot \hat{\mathbf{S}} | JM \right\rangle =$$
$$= \left\langle J'M' \left| \left(\hat{S}_i \hat{S}_i | \mathbb{J}_K \right) \right| JM \right\rangle = S(S+1)\delta_{MM'}$$

23 С другой стороны,

$$\left\langle JM' \left| \hat{S}_i \hat{S}_i \right| JM \right\rangle = \left\langle JM' \left| \Lambda^2(J) \hat{J}_i \hat{J}_i \right| JM \right\rangle =$$
$$= \Lambda^2(J) J(J+1) \delta_{MM'}.$$

Отсюда получаем другой результат: кажется, что фактор Ланде равен

$$g_{JLS}^{\text{wrong}} = 1 + \sqrt{\frac{S(S+1)}{J(J+1)}}.$$

Равенства (22) и, следовательно, (23) неверны. В самом деле, теорема Вигнера-Эккарта утверждает не пропорциональность операторов $\hat{S}_i$ и $\hat{J}_i$, а пропорциональность их матричных элементов на каждом $\mathbb{J}_K$:

$$\left\langle JM' \left| \hat{S}_i \hat{S}_i \right| JM \right\rangle =$$
$$= \sum_{J'', M''} \left\langle JM' \left| \hat{S}_i \right| J'', M'' \right\rangle \left\langle J'', M'' \left| \hat{S}_i \right| JM \right\rangle$$

Для применения теоремы Вигнера-Эккарта к матричным элементам в последнем равенстве нужно, чтобы операторы $\hat{S}_i$ рассматривались лишь на подпространствах $\mathbb{J}_K$. То есть чтобы матричные элементы сужения произведения операторов, записанного в левой части равенства (24), были равны матричным элементам произведения сужений операторов на $\mathbb{J}_K$ - правой части равенства (24). В Утверждении 17 показано, что это неверно. Соответственно, фактор Ланде не может быть вычислен с помощью рассмотрения матричных элементов $\hat{S}_i \hat{S}_i$.

10.3 Two- and Three-Body Problems

(??????????????????????????)

10.3.1 Separation of the Center of Mass

(из Киселева) $\frac{1}{2m_1}\boldsymbol{\nabla}_1^2+\frac{1}{2m_2}\boldsymbol{\nabla}_2^2=(\boldsymbol{\nabla}_1,\boldsymbol{\nabla}_2)\begin{pmatrix}\frac{1}{2m_1} & 0\\ 0 & \frac{1}{2m_2}\end{pmatrix}\cdot\begin{pmatrix}\boldsymbol{\nabla}_1\\ \boldsymbol{\nabla}_2\end{pmatrix}$

Рассмотрим оператор Шрёдингера для задачи двух тел (см. пример 2.2 в разделе 2.2.4 главы 2):

$$H=-\frac{\hbar^2}{2m_1}\Delta_1-\frac{\hbar^2}{2m_2}\Delta_2+V\left(x_1-x_2\right)$$

Вводя

$$\boldsymbol{X}=\frac{m_1\boldsymbol{x}_1+m_2\boldsymbol{x}_2}{m_1+m_2}\quad\text{и}\quad\boldsymbol{x}=\boldsymbol{x}_1-\boldsymbol{x}_2$$

координаты центра масс и относительную координату, получаем

$$H=-\frac{\hbar^2}{2M}\Delta_{\boldsymbol{X}}-\frac{\hbar^2}{2\mu}\Delta_{\boldsymbol{x}}+V(\boldsymbol{x})$$

где $M=m_1+m_2$ - полная масса, а $\mu=\frac{m_1m_2}{m_1+m_2}$ - приведенная масса.

Оператор Гамильтона H диагонализуется методом разделения переменных. Конкретно, рассмотрим следующее разложение двухчастичного гильбертова пространства $\mathscr{H}=L^2\left(\mathbb{R}^6\right)$ в тензорное произведение гильбертовых пространств:

$$\mathscr{H}=L^2\left(\mathbb{R}^3,d^3\boldsymbol{X}\right)\otimes L^2\left(\mathbb{R}^3,d^3\boldsymbol{x}\right)$$

Оператор

$$H_X=-\frac{\hbar^2}{2M}\Delta_{\boldsymbol{X}}$$

действует как тождественный на втором сомножителе в (4.1), а оператор

$$H_{\boldsymbol{x}}=-\frac{\hbar^2}{2\mu}\Delta_{\boldsymbol{x}}+V(\boldsymbol{x})$$

как тождественный оператор на первом сомножителе в (4.1). У функцийрешений задачи на собственные значения

$$H\psi=E\psi$$

имеющих вид произведения

$$\psi(\boldsymbol{X},\boldsymbol{x})=\Psi(\boldsymbol{X})\psi(\boldsymbol{x})$$

переменные разделяются:

$$H_{\boldsymbol{X}}\Psi(\boldsymbol{X})=E_1\Psi(\boldsymbol{X})\quad\text{и}\quad H_{\boldsymbol{x}}\psi(\boldsymbol{x})=E_2\psi(\boldsymbol{x})$$

где $E=E_1+E_2$. Поскольку

$$\Psi(\boldsymbol{X})=\left(\frac{1}{2\pi\hbar}\right)^{\frac{3}{2}}e^{\frac{i}{\hbar}\boldsymbol{k}\boldsymbol{X}},\quad\boldsymbol{k}^2=2ME_1,$$

квантовая задача двух тел сводится к задаче о квантовой частице, движущейся в потенциальном поле, и описывается оператором Гамильтона (4.3) в гильбертовом пространстве $L^2\left(\mathbb{R}^3,d^3x\right)$.

10.3.2 Connection with Two- and Three-Body Problem in Classical Mechanics

(??????????????)

11 Models of Relativistic QM and QFT

(тут большая теория по ней, однако прямо так углубляться не буду. чисто базовая вузовская программа)

11.1 Basics of QFT (Ch. IV in LL4)

(см. пока об этом в записи по КТП)

11.1.1 Particle in an External Field

(?? see Landau's book)

11.1.2 Dirac Equation for an Electron in an External Field

(?? see Landau's book)

11.1.3 Expansion in Powers of $1/c$

(?? see Landau's book)

11.1.4 Fine Structure of the Hydrogen Atom

(?? see Landau's book)

11.1.5 Motion in a Centrally Symmetric Field

(?? see Landau's book)

11.1.6 On Other Topics in Quantum Electrodynamics

Движение в кулоновом поле

Рассеяние в центрально-симметричном поле

Рассеяние в ультрарелятивистском случае

Система волновых функций непрерывного спектра для рассеяния в кулоновом поле

Электрон в поле плоской электромагнитной волны

Движение спина во внешнем поле

Рассеяние нейтронов в электрическом поле

11.2 Introduction to Particle Physics

(тут очень коротко и многое лишь как указание, потому что подробно все в отдельной записи.)

11.2.1 True Overview of Modern Particle Physics

(I'll write later what really happens in this field, it is not obvious.)

Overview of history of modern particle physics

(write what happened in it? which were the most important discoveries and where are we going?)

11.2.2 Standard Model: Basic Concepts

(just a summary of the note on Standard model)

11.2.3 Experiments of Particle Physics: Basics

детектирование частиц

(?? how is it done?)

О некоторых ускорителях

ATLAS

(??? write shortly what is it?)

12 Famous numerical methods

(see another notes for them. Many numerical methods are in scope of cond matter or statistical physisc)

12.0.1 Wolfram methods

(I'll write later, see a book about it, corrently, there was no time to master it)

12.0.2 QuSpin

Method from 2018. Later maybe I'll study it.

Part IV
Parts of Quantum Mechanics

(сюда многое перенесу из разделов выше, что не является типичным методом)

13 Estimations and Well-known Effects

13.1 Estimates in Atomic Mechanics

В этом разделе будут получены основные результаты атомной механики. Для получения соотношений мы будем использовать, кроме размерных, также модельные оценки. Идея модельных оценок состоит в рассмотрении предельных случаев и упрощенных вариантов задачи.

(!!!! это в 1ю часть во многом перенесу!!!)

13.1.1 Estimates of Velocities and Sizes of Inner Electron Orbits in the Atom

Для оценки скорости электрона на внутренней орбите атома нужно составить величину с размерностью скорости из величин, определяющих структуру атома, т. е. из массы электрона m, постоянной Планка $\hbar$ и произведения заряда ядра и заряда электрона $Ze \cdot e$. Действительно, в уравнение движения заряд электрона входит только в виде произведения на заряд ядра, поскольку при рассмотрении внутренних электронов влиянием других электронов можно пренебречь. Задача нерелятивистская, поэтому скорость света не войдет. Единственная величина размерности скорости, которую можно составить из $m, \hbar$ и $Ze^2 - 9v \subset \Omega e^2/\hbar$.

Для оценки порядка величины радиуса внутренних орбит электрона a воспользуемся тем, что потенциальная энергия электрона Ze^2/a порядка его кинетической энергии mv^2, т. е. $Ze^2/a \sim mv^2$ или $a \sim \hbar^2/Zme^2$. Из оценок α и v видно, что при рассмотрении атомных явлений удобны единицы $e = \hbar = m = 1$ (так называемые атомные единицы). В этих единицах скорость света $c = 137,2$, а масса протона $M = 1840$.

13.1.2 Stationary States

Яма

Рассмотрим движение частицы в потенциальной яме (рис. 10).

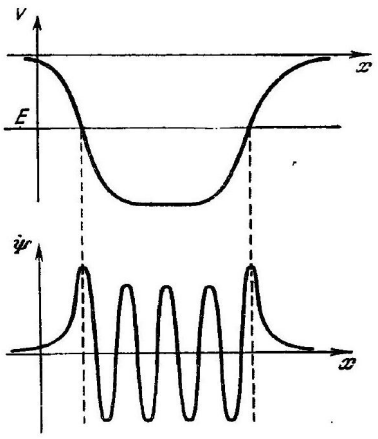


Рис. 10.

Уравнение Шредингера для этого случая имеет вид

$$\Psi'' + k^2\Psi = 0,$$

причем $k^2 = 2(E - V)$. В классически доступной области потенциальная энергия V меньше полной энергии E. Следовательно, волновая функция Ψ осциллирует в этой области (см. 1.1). В области, где $E < V$, Ψ-функция экспоненциально затухает. Энергию стационарных состояний можно оценить из условия, что характерный размер l области, в которой может двигаться частица, содержит целое число n полуволн де-Бройля.

Стационарные уровни энергин нельзя получить, исходя из одних лишь размерных соображений, так как величина n безразмерна. Мы будем делать модельные оценки, заменяя реальную потенциальную яму ящиком (рис. 11) с длиной, зависящей от энергии частицы.

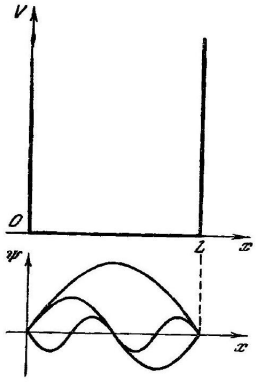


Рис. 11.

Длина де-Бройлевской волны

$$\lambda\!\!\!^{-} = 1/p = 1/\sqrt{2(E - V)},$$

где p - импульс частицы. Для произвольной потенциальной ямы λ зависит от координаты x. Для оценки всегда можно считать $\hbar \sim 1/\sqrt{2E}$, если E отсчитано от дна ямы.

Итак, оценка стационарных уровней системы E_n получается из соотношения

$$L\,(E_n) \approx \frac{n}{2}\lambda \sim \frac{2\pi n}{2\sqrt{2E_n}},$$

где $L\,(E_n)$ - характерная длина области, в которой может двигаться частица.

Для прямоугольной ямы величина $L\,(E_n) = L$ - длине ямы.

Следовательно, $L = \frac{\pi n}{\sqrt{2E_n}}$, откуда $E_n = \frac{\pi^2 n^2}{2L^2}$. Это выражение удовлетворяет принципу соответствия Бора: при больших квантовых числах расстояние между соседними энергетическими уровнями должно равняться классической частоте движения Действительно,

$$\frac{dE_n}{dn} = 2\frac{\pi^2 n}{2L^2} = \frac{\pi n}{L}\frac{2\pi}{2L} = \frac{2\pi}{2L/\frac{\pi n}{L}} = \frac{2\pi}{2L/v} = \frac{2\pi}{T_{\text{K}J}},$$

где $T_{\text{кл}}$ - классический период движення, равный $2L/v$.

Одномерный осциллятор

Следующий пример - одномерный осциллятор, потенциальная энергия которого $V = \frac{1}{2}\omega^2 x^2$. Здесь ω - частота классического осциллятора. Заметим, что частота осцилляций Ψ-функции около начала координат (рис. 12) больше, чем у краев ямы.

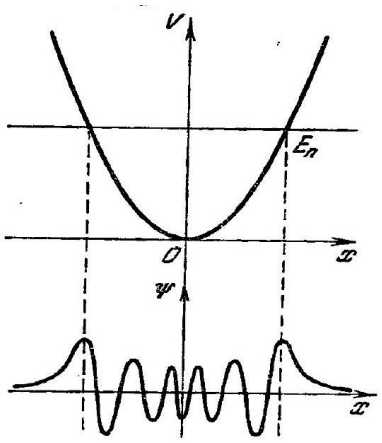


Рис. 12.

Действительно, при $x = 0$ кинетическая энергия движения максимальна, следовательно, длина волны k минимальна. При заданной энергии E_n характерная длина области L, в которой может двигаться частица, находится из условия $V(L) = E_n$. Итак, $\frac{1}{2}\omega^2 L_n^2 \sim E_n$, откуда $L_n \sim \sqrt{E_n}/\omega$. Условие квантования (1.27) имеет вид $\sqrt{E_n}/\omega \sim n/\sqrt{E_n}$, откуда $E_n = C_1 n\omega$. Из принципа соответствня следует, что $C_1 = 1$

Как известно, точное решение задачи приводит к спектру осциллятора $E_n = \left(n + \frac{1}{2}\right)\omega$, т. е. при $n = 0$ энергия колебаний отлична от нуля. Это связано с соотношением неопределенностей: частица, движущаяся в малой области d, не может иметь импульс, меньше $\sim 1/d$. Энергия E имеет оценку $E \sim \frac{1}{d^2} + \omega^2 d^2$. Возьмем минимум этого выражения. Эта минимизация соответствует вариационному принципу квантовой механики: $E = \min(\psi|H|\psi)$. В данном случае ψ-функция зависит от одного лишь параметра d. Выражение для E минимально при $d \sim 1/\sqrt{\omega}$. При этом $E_{\min} = C_2\omega\,(C_2 = 1/2)$. Величина $d^2_{\min} \sim 1/\omega$ дает оценку квадрата амплитуды нулевых колебаний.

Движение в кулоновском поле(!!??!?!)

Рассмотрим движение в кулоновском поле (рис. 13). Ограничимся случаем $l = 0$ (случай $l \neq 0$ будет рассмотрен квазиклассически на стр. 138).

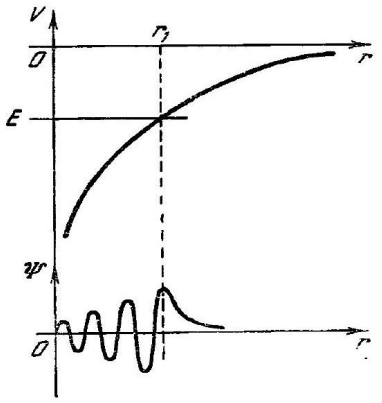


Рис. 13.

Существенная длина движения L находится из условия $E \sim Z/L$, т. е. $L \sim Z/E$. Из условия квантования (1.27) находим $Z/E_n \sim n/\sqrt{E_n}$, т. е. $E_n = C_1 \frac{Z^2}{n^2}$. Число C_1 найдем из принципа соответствия:

$$\frac{dE_n}{dn} = -C_1 \frac{2Z^2}{n^3} = \omega_{\text{К}\pi} = \frac{2\pi}{T_{\text{К}\pi}}.$$

Период классического движения

$$T_{\text{кл}} = 2\int_0^{r_1} \frac{dr}{v} = 2\int_0^{-Z/E} \frac{dr}{\sqrt{2\left(E_n + Z/r\right)}} = \frac{2\pi Z}{\left(2E_n\right)^{3/2}}.$$

Итак, $-C_1 \frac{2Z^2}{n^3} = \frac{2\pi}{2\pi Z}\left(-2C_1 \frac{Z^2}{n^2}\right)^{3/2}$, откуда $C_1 = -\frac{1}{2}$. Окончательно $E_n = -\frac{1}{2}\frac{Z^2}{n^2}$, что, как известно, совпадает с точным решением.

13.1.3 Distribution of Electric Charge in an Atom

Распределение заряда в тяжелых атомах можно вычислять с помощью приближенного метода, называемого методом Томаса-Ферми. При этом используется тот факт, что в тяжелом атоме большинство электронов имеет большие квантовые числа. Длины волн электронов при этом малы по сравнению с областью изменения потенциала. Тогда плотность электронов в каждой точке атома можно рассчитывать так же, как и плотность свободных электронов в потенциальном ящике с плоским дном.

Пусть наибольший импульс электронов в данной точке равен p_0. Тогда число состояний в интервале $(p, p+dp)$ равно $d\boldsymbol{p}/(2\pi)^3$. Поскольку в основном состоянии атома Электроны должны заполнять все состояния с импульсом, меньшим p_0, то число электронов в единице объема равно

$$n = 2\int \frac{dp}{(2\pi)^3} = 2\frac{4}{3}\pi p_0^3 \frac{1}{(2\pi)^8}$$

(множитель 2 возникает из-за двух возможных проекций спина электрона).

Обозначим через $\varphi(r)$ электростатический потенциал атомного поля. Согласно уравнению Пуассона

$$\Delta\varphi = 4\pi n,$$

Т. е.

$$\Delta\varphi \sim p_{0^3}.$$

Свяжем $p_0 c\varphi$. Полная энергия электрона равна $\frac{p^2}{2} - \varphi(r)$. Пусть $\varepsilon_0 \to$ максимальное значение полной энергии в каждой точке атома, т. е.

$$\varepsilon_0 = \frac{p_0^2}{2} - \varphi(r)$$

Величина ε_0 должна быть постоянной, иначе электроны будут переходить из точек с большей энергией в точки с меньшей энергией. Uз двух последних формул находим

$$\Delta\varphi \sim \left(\varphi + \varepsilon_0\right)^{3/2}$$

или

$$\Delta\varphi \sim \varphi^{3/2},$$

если отсчитывать ϕ от $-\varepsilon_0$.

Определим радиус l области, в которой находится большинство атомных электронов. Из последней формулы имеем по порядку величины

$$\frac{\varphi}{l^2} \sim \varphi^{3/2}, \text{ откуда } l \sim \varphi^{-1/4}.$$

С другой стороны, величину l можно связать с числом всех электронов атома Z:

$$Z \sim nl^3$$

или, учитывая соотношение $\Delta\varphi \sim p_0^8$,

$$Z \sim \Delta\varphi l^3 \sim \frac{\varphi}{l^2} l^3 \sim \varphi l.$$

Сравнивая два последних выражения, находим $Z \sim l^{-4} \cdot l$ или

$$l \sim \frac{1}{Z^{1/3}}.$$

(?????? почему????) Средняя энергия ε атомного электрона по порядку величины равна электростатическому потенциалу $\varphi(l)$. Так как $l \sim \varphi^{-1/4}$, то получаем

$$\varepsilon \sim l^{-4} \sim Z^{4/3}.$$

Полная энергия всех электронов E имеет порядок величины

$$E \sim \varepsilon Z \sim Z^{7/3}.$$

Число узлов волновой функции есть $l\sqrt{\varepsilon} \sim Z^{1/3}$.

Итак, радиус K, L-оболочки атома $r_K \sim 1/Z$, расстояние l (томас-фермиевский радиус) $\sim 1/Z1/3$ и радиус наружных оболочек ~ 1, поскольку эффективный зарлд для электронов наружных оболочек ~ 1.

Распределение электрического заряда в атоме рассматривается в разделе 3.2 подробнее. (?????)

13.1.4 Rutherford Formula

(???? это повторение механики??? в 1й части по механике скорее всего это же будет, мб чуть короче. пока тренироваться нужно!)

Рассмотрим рассеяние легкой частицы с массой m и зарядом e на тяжелой частице с зарядом Ze в нерелятивистском классическом случае.

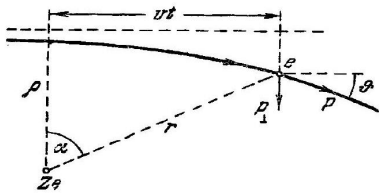


Рис. 14.

Сечение рассеяния не зависит от массы тяжелой частицы; оно определяется скоростью налетающсй частицы v, ее массой и зарядами e и Ze. Из закона Кулона следует бнлннейность сечения по зарядам, т. е. сечение σ будет зависеть лишь от комбинации Ze^2. Из этих параметров можно составить только одну величину с размерностьюдлины, а именно Ze^2/mv^2; следовательно, сечение рассеяния

$$\sigma(\theta) = \left(\frac{Ze^2}{mv^2}\right)^2 f(\theta)$$

Найдем зависимость сечения от угла рассеяния в предельном случае малых углов. Угол отклонения θ приближенно равен (рис. 14) $\theta \approx p_\perp/p$, где p-импульс частицы, а $p_\perp$ - импульс, возникающий в направлении, перпендикулярном к исходному. Вычислим $p_\perp$:

$$p_\perp = \int\limits_{-\infty}^{\infty} F_\perp dt = \int\limits_{-\infty}^{\infty} \frac{Ze^2}{r^2}\cos\alpha dt = \int\limits_{-\infty}^{\infty} \frac{Ze^2\rho dt}{(\rho^2+v^2t^2)^{3/2}} = \frac{2Ze^2}{\rho v}\int\limits_0^{\infty}\frac{dx}{(1+x^2)^{3/2}} = \frac{2Ze^2}{\rho v}$$

(интеграл берется сразу заменой $x = \operatorname{tg} y$); здесь ρ-прицельное расстояние (см. рис. 14). Следовательно,

$$\theta(\rho) = \frac{2Ze^2}{mv^2\rho}.$$

Го определению дифференциального сечения рассеяния:

$$d\sigma = \rho d\rho d\varphi = \rho\left|\frac{d\rho}{d\theta}\right| d\theta d\varphi = \rho\left|\frac{d\rho}{d\theta}\right|\frac{\sin\theta d\theta d\varphi}{\sin\theta},$$

или

$$\frac{d\sigma}{d\Omega} = \rho\left|\frac{d\rho}{d\theta}\right|\frac{1}{\sin\theta}$$

Используя (1.28) и (1.29), получаем формулу Резерфорда для малых углов рассеяния:

$$\frac{d\sigma}{d\Omega} = \left(\frac{2Ze^2}{mv^2}\right)^2\frac{1}{\theta^4}$$

13.1.5 Inapplicability of Classical Mechanics at Large Impact Parameters (!!!!!!!)

(!?!?!!? важный раздел, потом подумаю больше про него!!! в 1х частях укажу точно!)

В классической механике полное сечение рассеяния

$$\sigma = \int\limits_0^{\infty} 2\pi\rho d\rho$$

обращается в бесконечность для любых потенциалов (кроме обрывающихся, как, например, потенциал твердого иарика). В квантовой механике полное сечение конечно для потенциалов, убывающих с расстоянием быстрее, чем $1/r^2$ (см. задачу). Покажем, что классическая механика становится неприменимой при достаточно малых углах рассеяния, т. е. при достаточно больших прицельных параметрах о. Мы увидим, что с увеличением прицельного параметра угол квантовомеханической дифракции θ_d уменьшается медленнее, чем угол классинеского рассеяния θ. Поэтому, начиная с некоторого прицельного па- раметра ρ_1 угол θ_d становится больше $\theta_{\text{кл}}$.

Следовательно, дифференциальное сечение рассеяция для прицельных параметров рассеяиня, ббльших ρ_1, нужно рассчитывать по квантовомеханическим формулам. Итак, хотя длина волны λ здесь много меньше характерного размера, т. е. ρ_1, условия классичности рассеяния не выполняются, т. е. условие $\lambda \ll \rho_1$ - необходимое, но вовсе не догтаточное условие применимости классической механики. Получим критерий применимости классической меха ники. Согласно оценке $\theta \approx p_\perp/p$ заключаем, что

$\theta_{\text{КІ}} \sim F_\perp \Delta t/p \sim \frac{\partial V}{\partial \rho}\frac{\Delta t}{p} \sim \frac{V(\rho)}{p}\frac{\Delta t}{\rho} \sim \frac{V(\rho)}{pv}$, т. е. $\theta_{\kappa\Omega} \sim \frac{V(\rho)}{E}$. Здесь мы предположили, что $\frac{\partial V}{\partial \rho} \sim \frac{V}{\rho}$ (см. стр. 8) (E- энергия частицы, V - потенциал взаимодействия).

Для нахождения угла дифракции рассмотрим следующий опыт. Экран с отверстием диаметра a ограничивает прицельные параметры рассеяния значениями $\rho \pm a$ (рис. 15). Для применимости классической механики необходимо, чтобы ши-

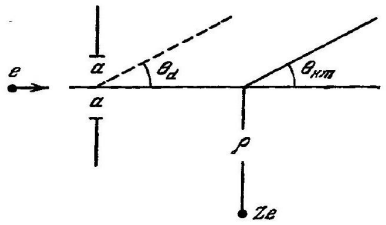


Рис. 15.

рина цели a была много меньше прицельного параметра ρ, иначе само понятие прицельного параметра теряет смысл. При сужении отверстия возникает дифракционное рассеяние. Чтобы можно было наблюдать отклонение, необходимо, чтобы дифракционный угол был много меньше угла рассеяния.

Из соотношения неопределенностей видно, что неопределенность в координате a соответствует неопределенности в поперечном импульсе $\Delta p \sim \hbar/a$. Следовательно, угол дифракции

$$\theta_d \sim \frac{\Delta p}{p} \sim \frac{1}{pa},$$

где p - импульс налетающей частицы. Для применимости классической механики необходимо, чтобы $\theta_{\text{cl}} \geqslant \theta_d$, или $\theta_{\text{cl}} \geqslant 1/pa$. Тем более,

$$\theta_{\text{cl}} = \frac{V(\rho)}{E} \geqslant \frac{1}{p\rho}.$$

Это-общий критерий применимости классической механики для задачи рассеяния. Для потенциалов, спадающих с расстоянием быстрее, чем кулоновский, классический угол рассеяния убывает с ростом прицельного параметра сильнее, чем $1/\rho$. Поэтому всегда найдется прицельный параметр ρ_1, для которого $\theta_{\text{кл}} \sim \theta_d$. В случае резерфордовского рассеяния $\theta = \frac{2Ze^2}{p\rho v}$ и рассеяние будет для всех углов классическим, если $Ze^2/\hbar v \gg 1$.

13.1.6 Estimate of Cross Sections for Potentials Decaying Faster than Coulomb (?????)

Мы получили, что классическая механика неприменима при прицельных параметрах, больших ρ_1, которое определяется из условия равенства классического угла рассеяния дифракционному:

$$\frac{\hbar}{\rho_1 p} = \theta_{\text{КІ}}(\rho_1),$$

т. е. величина ρ_1 находится из соотношения

$$\frac{\hbar}{\rho_1 p} \sim \frac{V(\rho_1)}{E}$$

)E - энергия налетающей частицы). Из (1.32) можно найти ρ_1 для любого конкретного вида потенциала $V(\rho)$, спадающего с расстоянием быстрее кулоновского (для последнего обе части соотношения (1.32) пропорциональны $1/\rho$, т. е. ρ_1 найти

нельзя). Следовательно, при $\rho < \rho_1$ дифференциальное сечение рассеяния можно вычислять по формулам классической механики.

Полное сечение рассеяния

$$\sigma = \pi\rho_1^2 + \sigma_{\text{диФ}} ,$$

где $\sigma_{\text{диф}}$ - дифракционное сечение рассеяния.

Если потенциал достаточно быстро убывает ($V(r) \underset{r\to\infty}{<} 1/r^2$, см. задачу), то сечение рассеяние может быть оценено как дифракционное сечение рассеяния на экране радиуса ρ_1, т. е. $\sigma_{\text{диф}}$ имеет порядок $\pi\rho_1^2$, так что

$$\sigma \sim 2\pi\rho_1^2.$$

Оценим полное сечение рассеяния для степенного потенциала $V = \alpha/r^n$. Из формулы (1.32) находим $\frac{1}{\rho_1 p} \sim \frac{\alpha}{\rho_1^n E}$, откуда $\rho_1 \sim (\alpha/v)^{\frac{1}{n-1}}$. Следовательно,

$$\sigma \sim 2\pi\rho_1^2 \sim 2\pi \left(\frac{\alpha}{i}\right)^{\frac{2}{n-1}} .$$

При n, близком к 2, эта оценка не годится (см. задачу).

З а дача. Определить, при какой степени убывания потенциала полное сечение рассеяния конечно.

13.1.7 Resonance Effects in Scattering (!!!!!)

Рассмотрим сначала рассеяние на потенциале, имеющем сильно отталкивающую сердцевину (рис. 16).

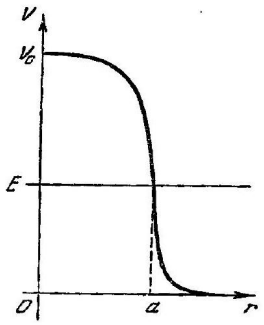


Рис. 16.

Обозначим через V_0 и a соответственно высоту и ширину потенциального барьера. Предположим, что $V_0 \gg E$-энергии налетающей частицы. Тогда на границе барьера волновая функция обращается в нуль: $\Psi(a) = 0$. Рассмотрим для простоты сферически - симметричное рассеяние и предположим, что при $r > a$ частица движется свободно, т. е. ее волновая функция есть сумма падающей плоской волны e^{ik2} и расходящейся сферической волны $\frac{f}{r}e^{ikr}$, где f-амплитуда рассеяния. Плоская волна e^{ikz} имеет сферически-симметричную часть, равную $\frac{\sin kr}{kr}$. Действительно, если разложить e^{ikz} в ряд по полиномам Лежандра: $e^{ikz} = e^{ikr\cos\theta} = \sum\limits_{l=0}^{\infty} f_l P_l(\cos\theta)$, то $f_0 = \frac{1}{2}\int\limits_0^{\pi} e^{ikr\cos\theta}\sin\theta d\theta = \frac{\sin kr}{kr}$. Итак,

$$\int \Psi \frac{d\Omega}{4\pi}\bigg|_{r>a} = \frac{\sin kr}{kr} + \frac{f_i}{r}e^{ikr}.$$

Используя граничное условие $\Psi(a) = 0$, находим $\frac{\sin ka}{k} + + fe^{ika} = 0$, или

$$f = -\frac{\sin ka}{k} e^{-ika}.$$

Если энергия частицы такова, что $ka = n\pi$, где n-пелое число, то $f = 0$, т. е. сечение s-рассеяния обращается в нуль. Этот резонансні:й эффект для отталкивательного потенциала ослаблен тем, что при $ka \geqslant 1$ в рассеянии существенны и волны с $l \neq 0$. Поэтому полное сечение рассеяния не обращается в нуль.

Как видно из выражения для амплитуды рассеяния, нанбольшее сечение получается при $ka = (2n+1)\frac{\pi}{2}$: $\sigma = 4\pi\star^2$. При малых $k(ka$

Резонансные эффекты при рассеянии используются в так называемой просветленной оптике: на поверхность линзы наносится слой вещества такой толщнны, чтобы разность фаз от слоя и линзы составила целое число . В результате на поверхности линзы не происходит отражения света и все потери обусловлены лишь поглощением.

Аналогичное явление происходит при рассеянии частиц на потенциальной яме ($V < 0$). Как и в случае $V > 0$, сечение рассеяния принимает различные значения в зависимости от фазы волновой функции у края ямы. При определенных значениях фазы сечение обрацаается в нуль. Этот эффект наблюдался впервые Рамзауэром при рассеянии электронов на атомах. Классическая теория рассеяния не может объяснить это явление. Другой пример, где классическая механика решительно противоречит эксперименту,- это захват медленных нейтронов ядрами. Сечение этого процесса ($\sim 4\pi\lambda^2$) превышает классическое сечение ($\sigma_{\text{кл}} = \pi R^2$, где R - радиус ядра) в десятки тысяч раз.

13.1.8 Interaction Between Atoms

Оценим величину взаимодействия нейтрального атома с ионом и с нейтральным атомом на больших расстояниях. Ион создает электрическое поле $E = Z_1/r^2$, где Z_1-заряд иона. Нейтральный атом, находящийся в электрическом поле E, приобретает дипольный момент $d = \alpha E$, где α-поляризуемость атома. Следовательно, взаимодействие иона с нейтральным атомом $V = -Ed = -Z_1^2\alpha/r^4$. В атомных единицах $\alpha \sim 1$, так как главную роль в поляризации атома играют наружные оболочки, для которых все величины ~ 1 в атомных единицах. Таким образом, $V \sim -Z_1^2/r^4$.

Рассмотрим теперь случай, когда оба атома нейтральны. Они индуцируют друг у друга дипольные моменты $\overline{d_1}$ и $\bar{d}_2$. Диполь-дипольное взаимодействие между атомами равно $V \sim -\vec{d}_1\vec{d}_2/r^3$

Среднее значение $\bar{d}_1$ и $\bar{d}_2$ по основному состоянию равно нулю, так как атомы не имеют постоянных дипольных моментов. Однако среднее значение $\bar{d}_1^2, \bar{d}_2^2$ отлично от нуля, так как дипольный момент колеблется со всеми возможными атомными частотами:

$$\bar{d} = \sum_\omega d_\omega e^{i\omega t}$$

Дипольный момент $d_{1\omega}$ создает поле $E_\omega \sim \frac{d_{1\omega}}{r^3}$. Момент $d_{2\omega}$ в этом поле равен $d_{2\omega} = \alpha_2 E_\omega$. Подставляя $d_{2\omega}$ в энергию взаимодействия, получим после усреднения по времени:

$$V \sim \sum_\omega d_{2\omega}E_\omega = -\frac{1}{r^6}\sum_\omega d_{1\omega}^2\alpha_2(\omega) \sim -\frac{1}{r^6}$$

13.1.9 Ionization of Atoms

Оценим потери энергии при движении быстрого электрона в газе. Налетающий электрон, сталкиваясь с электронами атомных оболочек, выбрасывает их из атома. При

большой энергии налетающего электрона его угол отклонения $\boldsymbol{v}$ мал. Поэтому сечение рассеяния на одном электроне оболочки определяется формулой $\frac{d\sigma}{d\Omega} \sim \frac{1}{p^4\vartheta^4}$; здесь p - импульс электрона.

Обозначим через q изменение импульса налетающего электрона; величина q связана с углом рассеяния $\forall$ соотношением $q \sim p\theta$. Энергия ΔE, передаваемая при столкновении, равна $q^2/2$. Потеря энергии электрона на единице длины пути равна:

$$\frac{dE}{dx} = -nZ \int \Delta E d\sigma,$$

где nZ - полное число электронов в единице объема, $d\sigma$ - дифференциальное сечение. Имеем:

$-\frac{dE}{dx} \sim Zn \int q^2 \frac{1}{p^4} \frac{1}{\vartheta^4} \vartheta d\vartheta =$

$$= Zn \int q^2 \frac{1}{p^4} \frac{p^2 dq}{q^3} = Zn \frac{1}{p^2} \int \frac{dq}{q} = \frac{Zn}{p^2} \ln \frac{q_{\max}}{q_{\min}}.$$

Максимальный классический угол отклонения $\vartheta^{\text{кл}}_{\max} \sim 1$, но он соответствует прицельным параметрам, много меньшим длины волны налетающей частицы. Такие прицельные параметры квантовомеханически бессмысленны. Минимальный прицельный параметр, о котором можно говорить в квантовой механике, имеет порядок длины волны λ. Отсюда $\vartheta_{\max} \sim \frac{1}{\rho_{\min} E} \sim \frac{1}{p}$ и $q_{\max} \sim p\vartheta_{\max} \sim 1$.

Минимальный передаваемый импульс соответствует случаю, когда время пролета электрона τ сравнивается с собственными временами (обратными частотами) атома $1/\omega_0$. При больших временах пролета поле налетающего электрона не содержит фурье-компонент с атомными частотами и вероятность ионизации резко убывает. Величина $\tau \sim \rho/\tau$, где v-скорость налетающего электрона. Итак, $q_{\min}$ находится из условия $\frac{\rho}{v} \sim \frac{1}{\omega_0}$. Так как $\boldsymbol{\vartheta} \sim 1/\rho E$, то $\vartheta_{\min} \sim \omega_0/vE$, а $q_{\min} \sim p\vartheta_{\min} \sim p\omega_0/vE \sim \omega_0/p^2$. Следовательно,

$$-\frac{dE}{dx} \sim \frac{Zn}{p^2} \ln \frac{p^2}{\omega_0}.$$

Как мы видели (см. стр. 36), основная масса электронов атома расположена в области радиуса $a_0/Z^{1/s}$ и энергия каждого из них $\sim Z^{4/3}$. Величина ω_0 имеет порядок $v/a \sim Z^2 !_3 / Z^{-1/3} \sim Z$. Поэтому

$$-\frac{dE}{dx} \sim \frac{Zn}{p^2} \ln \frac{p^2}{Z}.$$

13.1.10 Multiple Scattering

Узкий пучок электронов при прохождении через среду размывается по углам из-за многократного рассеяния. Действительно, хотя отклонение электрона, скажем, направо и налево, равновероятно, средний квадрат угла отклонения отличен от нуля.

С аналогичным явлением встречаются люди, имеющие телефон с трубкой телефона на шнуре, в обыденной жизни, наблюдая, как закручивается со временем этот шнур. При каждом телефонном разговоре шнур закручивается в ту или иную сторону равновероятно. Однако после больного числа разговоров шнур оказывается закрученным на угол, пропорциональный квадратному корню из числа разговоров. (????? что?? подумаю про это когда-то не скоро.)

Поскольку разброс электронов пучка по углам представляет собой совокупность большого числа независимых случайных процессов, то распределение по углам имеет

вид $\Phi(\vartheta) = Ae^{-\vartheta^2/\bar{\vartheta}^2}$ (гауссово распределение). Средний квадрат угла отклонения $\overline{\vartheta^2}$ пропорционален числу столкновений N, равному отношению толщины образца L к длине свободного пробега h. Если $\overline{\$_1^2}$ - средний квадрат угла отклонения при одном столкновении, то

$$\overline{\vartheta^2} = \overline{\vartheta_1^2}N = \overline{\vartheta_1^2}\frac{L}{l} = n\sigma L\overline{\vartheta_1^2} = \overline{0^2}L,$$

где σ-сечение рассеяния, n-число ядер в единице объема, а $\overline{\theta^2}$ - средний квадрат угла отклонения на единице длины пути, т. е. $\overline{\theta^2} = n\sigma\overline{\vartheta_1^2}$. Так как, по определению, $\overline{\vartheta_1^2} = \frac{1}{\sigma}\int \sigma(\vartheta)\vartheta^2 a\Omega$, то $\overline{\theta^2} = n\int \sigma(\vartheta)\vartheta^2 d\Omega$.

Для резерфордовского рассеяния получаем

$$\overline{\theta^2} \sim 2\pi n\frac{Z^2}{E^2}\ln\frac{\vartheta_{\max}}{\vartheta_{\min}}.$$

Эта формула годится как в релятивистском, так и в нерелятивнстском случае.

Рассмотрим два предельных случая: $Ze^2/\hbar v \gg 1$ и $2e^2/\hbar v \ll 1$. В первом случае рассеяние для всех углов можно считать классическим (см. стр. 40). Максимальный угол рассеяния определяется из условня, что прицельный параметр равен радиусу ядра R, т. е. $\vartheta_{\max} \sim V(R)/E = Z/RE$. Однако в случае рассеяния электронов значение $E \geqslant Z/R$ противоречит условию классичности; в обратном случае, который соответствует условию $Z/RE > 1, \dot{\vartheta}_{\max} \sim 1$. Минимальный угол отклонения определяется атомными размерами $a : \dot{\vartheta}_{\min} \sim Z/aE$. Оцценная а по модели Томаса-Ферми, находим $\vartheta_{\min} \sim Z/Z^{-1_{i3}}E \sim Z^4/E$. Следовательно, для электронов с $E < Z/R$

$$\overline{\vartheta^2} \sim 2\pi n\frac{Z^2}{E^2}\ln\frac{E}{Z^{4/3}}.$$

В случае, когда $Ze^2/\hbar v \ll 1$, классический угол отклонения меньше угла квантовомеханической дифракции ϑ_d. Поэтому углы $\vartheta_{\max}$ и $\vartheta_{\min}$ должны определяться следующим образом: $\vartheta_{\min}$ - угол дифракции на радиусе атома:

$$\vartheta_{\min} \sim \frac{\hbar}{a} \sim \frac{Z^{1/3}}{p}.$$

Тут $\vartheta_{\max}$ - угол дифракции на ядре:

$$\vartheta_{\max} \sim \frac{\hbar}{R} \sim \frac{1}{pR} \text{ при } \frac{\lambda}{R} < 1,$$
$$\vartheta_{\max} \sim 1 \quad \text{при } \frac{\lambda}{R} > 1.$$

Таким образом, в случае $Ze^2/\hbar v$

$$\overline{\theta^2} = 2\pi n\frac{Z^2}{E^2} \times \begin{cases} \ln\frac{a}{R}, & \lambda/R < 1, \\ \ln\frac{a}{\hbar}, & \star/R > 1. \end{cases}$$

13.2 Estimations and Effects in Quantum Electrodynamics

13.2.1 Zero Fluctuations of the Electromagnetic Field

Как известно, энергия электромагнитного поля равна $\int\left(\frac{\mathcal{E}^2}{8\pi} + \frac{g^2}{8\pi}\right)dr$, где $\mathscr{O}$ и $\mathscr{H}$ - напряженности электрического и магнитного полей. Если в пространстве нет зарядов, то

электростатический потенциал φ можно считать равным нулю. Тогда $\mathscr{E} = -\frac{1}{c}\frac{\partial A}{\partial t}, \mathscr{H} = \operatorname{rot} A$, где A - векторный потенциал.

Разложим векторный потенциал по плоским волнам:

$$A = \sum_{\boldsymbol{k}} A_k e^{ikr} + \text{ компл. сопряж.}$$

Тогда для энергии электромагнитного поля E получаем следующее выражение:

$$E = \sum_k \left\{ \frac{1}{8\pi c^2} \left|\dot{A}_k\right|^2 + \frac{k^2}{8\pi} \left|\dot{A}_k\right|^2 \right\}.$$

Здесь нормировочнын объем пространства, в котором находится поле, считается равным 1.

Легко видеть отсюда, что энергия электромагнитного поля равна сумме энергий невзаимодействующих гармонических осцилляторов. Действительно, величина $A_{\boldsymbol{k}}$ играет здесь роль координаты, $\dot{A}_k$ - скорости, $1/4\pi c^2$ - массы гармонического осциллятора. Частота осциллятора $\omega_k = \sqrt{\frac{\alpha}{m}}$, где α - жесткость, а m - масса. данном случае $\alpha = k^2/4\pi, m = 1/4\pi c^2$, следовательно, $\omega_k = ck$. Первое слагаемое в выражении (1.33) представляет собой кинетическуюо энергию электромагнитного поля, а второе-потенциальную.

Итак, электромагнитное поле в пространстве без зарядов можно рассматривать как совокупность независимых гармонических осцилляторов со всеми возможными значениями волнового вектора k.

ГПриеним к совокупности гармонических осцилляторов законы квантовой механики. Тогда энергия электромагнитного поля равна

$$E = \sum_k \left(n_k + \frac{1}{2}\right) \omega_k,$$

где n_k - номер возбужденного состояния осциллятора с волновым вектором k (число квантов с волновым вектором k). Для простоты здесь опускается значок λ поляризации кванта. Он определяет направление ориентации вектора A_k, лежаиего в плоскости, перпендикулярной к k. 8 основном состоянит все $n_k = 0$ (нет квантов) и $E = \frac{1}{2}\sum_k \omega_k$. При этом ни кинетическая, ни потенциальная. энергии колебаний не имеет определенного значения.

Следовательно, ни напряженность электрического поля, ни напряженность магнитного поля не имеют определенного значения. Средние значения электрического и магнитного полей при этом равны нулю, но средние значения от квадратов этих величин отличны от нуля. Это означает, что электромагнитное поле в пустоте колеблется. Эти колебания называются нулевыми колебаниями электромагнитного поля.

Теперь можно ответить на следующий вопрос: почему атомы не находятся неограниченно долго в возбужденных состояниях? Ведь возбужденные состояння есть точные стационарные состояния уравнения Шредингера. Причина заключается в том, цто в пустоте всегда есть электромагнитное поле, с которым взанмодействует атом. В результате состояния атома перестают быть стационарными.

Рассмотрим взаимодействие частицы с электромагнитным полем. Для того чтобы найти изменение гамильтониана при наложении поля, нужно импульс частицы p заменить на $p - \frac{e}{c}A$, где A - векторный потенциал поля. Следовательно, оператор кннетической энергии $\frac{p^2}{2m}$ преобразуется в $\frac{p^2}{2m} - \frac{e}{mc}pA + \frac{e^2}{2mc^2}A^2$. Последнее слагаемое в

этом выражении мало. Его нужно учитывать в задачах, где первый порядок теории возмущений дает нулевой вклад, например, в задаче рассеяния кванта на электроне. Операторы A_k играют роль координаты соответствующего осциллятора поля и поэтому имеют матричные элементы, соответствующие изменению числа квантов на 1.

Вычислим матричный элемент $(A_k)_{01}$ перехода из вакуумного состояния в состояние с одним квантом. Для этого найдем величину $(A_k^2)_{00} = \sum_n (0\,|A_k|\,nj)\,(n\,|A_k|\,0)$. Так как оператор A_k рождает один квант (с частотой ω_k), то в сумме отличен от нуля только член с $n = 1$. Итак, $|(A_k)_{01}| = \sqrt{\left(|A_k|^2\right)_{00}}$ Для гармонического осциллятора средние значения кинетической и потенциальной энергий совпалают и равны половине полной энергии. Следовательно, для основного состояния $\bar{T}_k = \bar{U}_k = \frac{1}{2}E_k = \frac{1}{4}ck$. Так как $\bar{U}_k = \frac{k^2}{8\pi}\left(|A_k|^2\right)_{00}$, то $\frac{1}{4}ck = \frac{k^2}{8\pi}\left(|A_k|^2\right)_{00}$, откуда $(A_k^2)_{00} = \frac{2\pi c}{k}$. Следовательно,

$$|(A_k)_{01}| = \sqrt{\frac{2\pi c}{k}} = \sqrt{\frac{2\pi c^2}{\omega_k}}.$$

Аналогично находится матричный элемент от A_k для перехода из состояния с n квантами в состояние с $n+1$ квантами.

Таким образом, матричный элемент перехода частицы из состояния φ_{λ_1} в состояние φ_{λ_2} с испусканием кванта равен

$$V_{\lambda_1\lambda_2} = \left(-\frac{ep}{mc}A_k\right)_{\lambda_1\lambda_2} = -\frac{e}{mc}\left(\varphi_{\lambda_1}\left|p\eta_{k\lambda}e^{ikr}\right|\varphi_{\lambda_2}\right)\sqrt{\frac{2\pi c^2}{\omega_k}}.$$

Чтобы перейти к релятивистскому случаю, достаточно для оценки заменить $\boldsymbol{p}/m$ на $\boldsymbol{v}$. Здесь $\boldsymbol{p}\eta_{k\lambda}$ - проекция импульса на направление $\boldsymbol{A_k}$ ($\eta_{k\lambda}$ - единичный вектор поляризации кванта).

13.2.2 Photoelectric Effect

Рассмотрим фотоэффект: квант света поглощается атомом, в результате чего из атома вылетает электрон. Число переходов за единицу времени равно $\frac{2\pi}{\hbar}\left|V_{\lambda_1\lambda_3}\right|^2 \times \delta\left(E_i - E_f\right)$, где E_i - энергия начального состояния, равная сумме энергий кванта ω_k и энергии электрона в начальном состоянии ε_{λ_1}, а $E_f = \varepsilon_p$ - энергия вылетевшего электрона. Число переходов электрона за единицу времени в состояния с импульсами $\boldsymbol{p}$ в интервале $[\boldsymbol{p}, \boldsymbol{p} + d\boldsymbol{p}]$ равно

$$\begin{aligned} dW &= 2\pi \int |V_{12}|^2\,\delta\left(\varepsilon_{\lambda_1} + \omega_k - \varepsilon_{\lambda_2}\right)\frac{dp}{(2\pi)^3} = \\ &= 2\pi \int |V_{12}|^2\,\frac{p^2\frac{dp}{dE}dE}{(2\pi)^3}\delta\left(\varepsilon_{\lambda_1} + \omega_k - \varepsilon_{\lambda_2}\right)d\Omega = \\ &= \frac{1}{(2\pi)^2}\int |V_{12}|^2\,\frac{p^2}{v}d\Omega. \end{aligned}$$

Сечение фотоэффекта равно отношению числа переходов за единицу времени к интенсивности потока квантов. Последняя равна скорости кванта c, так как в нормировочном объеме ($= 1$) находится один квант. Следовательно, по порядку величины имеем

$$\sigma \sim \frac{4\pi p}{(2\pi)^2 c}\left|V_{12}\right|^2.$$

Покажем, что в выражении (1.34) экспоненту e^{ikr} можно заменить единицей. Действительно, волновое число $k = \omega/c \sim I/c$, где I - потенциал ионизации атома; $I \sim Z^2$ для внутренних электронных оболочек. Радиус этих оболочек $\sim 1/Z$, следовательно, $kr \sim \frac{Z^2}{c}\frac{1}{Z} \sim \frac{Z}{c} \ll 1$ и $e^{ikr} \approx 1$. Экспоненту e^{ikr} тем более можно заменить единицей для наружных оболочек, где $kr \sim 1/c = 1/137$.

Так как $(\varphi_{\lambda_2} p \varphi_{\lambda_2}) = (\varphi\lambda_1 r \varphi\lambda_2) = i\left(\varepsilon_{\lambda_1} - \varepsilon_{\lambda_2}\right)(\varphi_{\lambda_1} r \varphi\lambda_2) = i\omega\left(\varphi_{\lambda_1} r \varphi_{\lambda_2}\right)$, то сечение фотоэффекта имеет порядок величины

$$\sigma \sim \frac{p}{c}\omega^2 \left|(\varphi_0 r \varphi_p)\right|^2 \frac{1}{\omega} \sim \frac{p\omega}{c}\left|(\varphi_0 r \varphi_p)\right|^2 .$$

Рассмотрим фотоионизацию K-оболочки в двух предельных случаях, когда энергия вылетающего электрона много меньше потенциала ионизации и когда она много больше потенциала ионизации. В первом случае энергия кванта близка к энергии ионизации $I \sim Z^2$, т. е.

$$\sigma \sim \frac{pZ^2}{c}\left|(\varphi_0 r \varphi_p)\right|^2 .$$

Возле порога реакции это сечение содержит множитель $p \sim \sqrt{E}$. Если бы матричный элемент r_{0p} не зависел от энергии, то $\sigma \sim \sqrt{E}$. Это-обычный результат для сечения реакций вблизи порога. Зависимость сечения $\sim \sqrt{E}$ возиикла из-за статистического веса конечных состояний:

$$\int \delta(E-\omega)\frac{dp}{(2\pi)^3} \sim \int \delta(E-\omega)p^2 dp \sim \int \delta(E-\omega)pdE \sim p.$$

В случае водородоподобного атома дело обстоит иначе: сечение фотоэффекта при малых энергиях вылетающего электрона не зависит от энергии. Это связано с тем, что дипольный матричный элемент из-за корневой особенности кулоновских волновых функций при $r^2 = 0$ (см. стр. 26) ведет себя как $1/\sqrt{p}$ вблизи порога реакции. Оценим r_{op} вблизи порога.

Волновая функция K-электрона $\varphi_0 \sim e^{-zr}$, и, следовательно, в дипольном матричном элементе существенны малые расстояння $r \sim 1/Z$. Для вылетевшего электрона волновая функция на большом расстоянии от ядра имеет вид плоской волны

$$\varphi_p = e^{ipr}.$$

Таким образом, чтобы оценить r_{0p}, нужно иайти φ_p при $r \sim 1/Z$. Для этого напишем уравнение Шредингера для радиальной части волновой функции $u_p/r : u_p'' + k^2 u_p = 0$, где $k^2 = 2(E + Z/r)$. В 1.1 мы получили следующее приближенное решение этого уравнения (так называемое квазиклассическое решение):

$$u_p = \frac{A}{\sqrt{k}}\cos\left(\int_{r_1}^{r} k dr - \frac{\pi}{4}\right), k = \sqrt{2(E+Z/r)}.$$

Здесь E-энергия вылетающего электрона на бесконечности, т. е. очень маленькая величина. Условия применимости (1.36) : $\frac{d\lambda}{dr} \ll 1$ (см. 1.1 и 3.1); отсюда получаем: $\frac{d\lambda}{dr} \sim 1/\sqrt{Zr}$, и условие квазиклассичности движения имеет вид $Zr > 1$, т. е. $r > 1/Z$. Итак, условие квазиклассичности движения выполняется вплоть до K-оболочки атома. Оценим нормировочный множитель A. Для этого рассмотрим u_p на больших расстояниях r:

$$u_p \approx \frac{A}{\sqrt[4]{2E}} \cos(pr + \alpha).$$

С другой стороны, при $r \to \infty$ волновая функция u_p/r должна совпадать с радиальной частью первой гармоники (оператор $\boldsymbol{r}$ меняет момент на 1) разложения плоской волны e^{ipr} по полиномам Лежандра: $e^{ipr\cos\theta} = \sum\limits_l f_l P_l(\cos\theta)$, амплитуда которой $\sim 1/pr$. Следовательно, из (1.36) находим: $A/\sqrt{p} \sim 1/p$, откуда $A \sim 1/\sqrt{p}$. Итак, волновая функция вылетевшего электрона φp при $r \sim 1/Z$ имеет оценку $\frac{1/\sqrt{p}}{r\sqrt[4]{Z/r}} \sim \frac{\sqrt{Z}}{\sqrt{p}}$.

Дипольныӈ матричный элемент $(\varphi_0 r \varphi_p)$ имеет порядок $(\varphi_0 \Gamma \varphi_p) \sim Z^3/2 \int\limits_0^\infty e^{-Zr} r \frac{\sqrt{Z}}{\sqrt{p}} r^2 dr \sim \frac{Z^2}{Z^4\sqrt{p}} \sim \frac{1}{Z^2\sqrt{p}}$.

Так как квадрат дипольного матричного элемента обратно пропорционален корню из энергии вылетающего электрона E, то сечение фотоэффекта σ не зависит от энергии E. Итак, при $E - I \ll I$ полное сечение фотоэффекта

$$\sigma \sim \frac{pZ^2}{c} \left(\frac{1}{Z^2}\right)^2 \frac{1}{p},$$

или

$$\sigma = \frac{C_1}{cZ^2}.$$

Рассмотрим другой предельный случай, когда энергия вылетающего электрона много больше потенциала ионизации. Оценим дипольный матричный элемент и сечение фотоэффекта. Волновая функция непрерывного спектра имеет вид $\varphi_p \underset{r\to\infty}{=} Fe^{ipr}$, где F - функция, стремящаяся к единице при $pr \gg 1$. В матричном элементе $(\varphi_0 p_0)$, как мы увидим, существенны расстояния $r \sim 1/p$. Отклонение F от единицы определяется величиной $V(r)/E$. При $r \sim 1/p$ можно полагать $F \approx 1$. Тогда в интеграле $(\varphi_0 p \varphi_p)$ оператор $\boldsymbol{p}$ можно вынести из-нод знака интеграла, заменив его числом p. Учет поляризации квантов внесет лишь множитель порядка 1. Следовательно,

$$\sigma \sim \frac{p}{c} |(\varphi_0 p \varphi_p)|^2 \sim \frac{p^2}{c} \left|\left(\varphi_0 e^{ipr}\right)\right|^2.$$

Интегрируя по углам, получаем

$$\left(\varphi_0 e^{ipr}\right) \sim Z^{3/2} \int_0^\infty e^{-Zr} \frac{\sin pr}{pr} r^2 dr = \frac{Z^{3/2}}{2p} \int_{-\infty}^\infty r e^{-Z|r|} \sin pr dr.$$

Оценим это выражение. Легко видеть, что вторая производная от функции $f(r) = re^{-Z|r|}$ имеет скачок при $r = 0$. Поэтому далекие фурье-компоненты этой функции имеют оценку (см. 1.1) $\sim Z/p^3$.

Если бы потенциал V как функция r^2 не имел особых точек на вещественной оси, то волновая функция как скаляр была бы аналитической функцией r^2. В этом случае далекая фурье-комнонента волновой функции как функция энергии была бы экспоненциально мала (см. 1.1). Мы видим, что степенная зависимость матричного элемента от энергии в нашем случае возникает из-за того, что Ψ в кулоновском потенциале как функция r^2 имеет точку ветвления при $r^2 = 0$. Эго связано с тем, что кулоновский потенциал $1/r$ имеет особенность при $r = 0$. Полюсная особенность кулоновского потенциала привела к корневой особенности в ренении уравнения Шредингера.

Iгак, матричный элемент $(\varphi_0 e^{ipr})$ при $p \to \infty$ имеет оленку $Z^{5/2}/p^4$, а сечение фотозффекта.

$$\sigma \sim \frac{Z^5 p}{cp^8}, \text{ т. е. } \sigma = \frac{C_2 Z^5}{cE^{7/2}}, \quad \text{или} \quad \sigma = \frac{2^{7/2} C_2}{cZ^2}\left(\frac{I}{E}\right)^{7/2}.$$

Здесь I-потенциал ионизации K-электрона, равный $Z^2/2$. Численный расчет показывает, что $C_2 \sim 10$.

Если положить в (1.39) энергию кванта E равной потенциалу ионизации I, то мы должны получить по порядку величины формулу (1.38). Однако, как показывают численные расчеты, формула (1.39) дает при $E = I$ сечение, на порядок большее, чем (1.38). Это означает, что переход от области $E - I \ll I$ к области $E \gg I$ оказывается сильно растянутым.

13.2.3 Lifetimes of Excited Atomic States

а) Оценим время жизни состояния $2p$ водородоподобного атома.

Электрон из состояния $2p$ переходит в состояние $1s$, испуская дипольный γ-квант. Число переходов в единицу времени (обратное время жизни) равно

$$W_{01} = 2\pi \int |V_{01}|^2 \frac{dk}{(2\pi)^3} \delta\left(E_0 - E_1 - \omega\right)$$

где $V = -\frac{1}{c} pA$ - потенциал взаимодействия электрона с электромагнитным полем. Индекс 0 соответствует состоянию $1s$, индекс 1 -состоянию $2p, \omega$ энергия γ-кванта. Так как

$$dk = k^2 dk d\Omega = k^2 \frac{dk}{d\omega} d\Omega d\omega$$

то

$$W_{01} = 2\pi \int |V_{01}|^2 \frac{k^2 \frac{dk}{d\omega} d\Omega}{(2\pi)^3}$$

Оценим матричиый элемент перехода V_{01}; учитывая нормировку потенциала A электромагнитного поля (см. стр. 49), находим

$$V_{01} = -\frac{1}{c}(p.A)_{01} \sim \sqrt{\frac{2\pi}{\omega}} p_{01}$$

Здесь мы не интересуемся поляризацией γ-кванта, которая внесет лишь численные множители. Оценим матричный элемент импульса p:

$$p_{01} = i\omega r_{01} \sim \frac{\omega}{Z}$$

$$W_{01} \sim \frac{\omega^2}{Z^2} \frac{1}{\omega} k^2 \frac{dk}{d\omega} \sim \frac{\omega^3}{Z^2 c^3}.$$

Следовательно,

Так как частота перехода имеет иорядок Z^2, то окончательно находим

$$W_{01} \sim \frac{Z^q}{c^3}$$

Оценим численно время жизни состояния относительно дипольного перехода. Атомное время жизни имеет порядок

$$\tau_{\text{at}} \sim \frac{\hbar}{E_{\text{at}}} \sim \frac{10^{-27} spz \cdot ce\kappa}{27s8 \cdot 1,6 \cdot 10^{-12} \text{ erg/eV}} = 0,3 \cdot 10^{-16}\text{s}.$$

Следовательно, $\tau_{\text{дип}} \sim \frac{c^9}{Z^4}\tau_{\text{ат}}$. Для атома водорода $\tau_{\text{дип}} \sim 10^7 \cdot 10^{-17} = 10^{-10}$ сек. Точный расчет дает несколько большие значения $\tau_{\text{дип}}$.

б) Оценим время жизни квадрупольных переходов, например, $3d \to 1s$**.**

Ранее в операторе A электромагнитного поля мы заменяли множитель e^{ikr} ($\boldsymbol{k}$-волновой вектор кванта) единицей $\left(kr = \frac{\omega}{c}r \sim \frac{Z}{c} \ll 1\right)$. При рассмотрении квадрупольных переходов нужно разложить e^{ikr} в ряд, Причем главный вклад внесет член разложения $i\boldsymbol{kr}$. Получаем

$$V_{01} = i\sqrt{\frac{2\pi}{\omega}}((\eta p)(kr))_{01},$$

где $\boldsymbol{\eta}$-поляризация кванта.

Направим ось z по вектору η, а ось x - по k (вектор поляризации кванта $\geqslant$ перпендикулярен к волиовому вектору k). Тогда

$$\begin{aligned} V_{01} = ik \quad & \sqrt{\frac{2\pi}{\omega}}\,(p_z x)_{01} = \\ & = ik\sqrt{\frac{2\pi}{\omega}}\left[\frac{1}{2}\,(p_z x - p_x z) + \frac{1}{2}\,(p_z x + p_x z)\right]_{01} = \\ & = ik\sqrt{\frac{2\pi}{\omega}}\left[-\frac{1}{2}[rp]_y + \frac{1}{2}\frac{d}{dt}(zx)\right]_{01}. \end{aligned}$$

Гервое слагаемое в этом выражении представляет собой матричный элемент от y-проекции момента количества дывижения, т. е. соответствует дипольному магнитному переходу. Произведение zx - это компонента квадрупольного момента, т. е. второе слагаемое определяет вероятность квадрупольного электрического перехода. Оба слагаемых имеют одинаковый порядок величины.

Оценим численно время жизни состояния относительно квадрупольного перехода. В отличие от дипольных переходов, в матричный элемепт добавляется множитель kr. Следовательно,

$$\tau_{\text{квад}} \sim \tau_{\text{дип}}\,\frac{1}{(kr)^2} \sim \tau_{\text{дип}}\,\frac{c^2}{Z^2}.$$

Для атома водорода $\tau_{\text{квад}} \sim 10^{-10} \cdot 10^4 \sim 10^{-6}$се.

З а д ач а.

Оценить время жизни водородоподобного атома по отношению к испусканию двух квантов. (!!??!?!?!?)

О т в е т. $\tau \sim c^6/Z^6$.

(хорошая задача, подумаю потом там!)

13.2.4 Braking radiation (!?!?)

(this is a big fundamental topic, I'll definetely create later several sections for it)

Оценим эффективное сечение излучения γ-квантов при рассеянии электронов иа ядре. Предположим, что частота φ-квантов много меньше энергии электрона. Тогда излучение слабо влияет на движение электрона и эффективное сечение приближенно равно произведению сечения рассеяния электрона на вероятность испускания γ-кванта.

Оценим вероятность испускания фотона при заданном дывижнии электрона. Уравнение Шрредингера для фотона в энергетическом представлении имеет вид

$$i\dot{C}_n = \sum_{n'} V_{nn'} C_{n'} e^{i(\omega_n - \omega_{n'})t},$$

где V описывает взаимодействие электрона с электромагнитным полем, а C_n - амплитуда состояния с n квантами с заданными волновым вектором и поляризацией.

В основном состоянии $C_0 = 1$, а все $C_n = 0$. В первом порядке теории возмущений отлична от нуля амплитуда перехода в состояние c одним квантом, C_1. Из (1.40) получаем

$$i\dot{C}_1 = V_{10} e^{i\omega t},$$

откуда

$$C_1 = -i \int\limits_{-\infty}^{\infty} V_{10} e^{i\omega t} dt = +i \int\limits_{-\infty}^{\infty} \left(\frac{1}{c} v A\right)_{10} e^{i\omega t} dt.$$

Мы написали взаимодействие с излучением для бесспиновых частиц. Для частиц со спином взаимодействие усложняется, но по порядку величины может быть оценено по этой же формуле.

Поскольку излучение не влияет на рассеяние электрона, то скорость v можно считать заданной функцией времени. Следовательно, так как $A \sim \eta e^{-ikr} \approx \eta e^{-i\omega \cdot \frac{\partial n}{c} t}$, то

$$C_1 = i\sqrt{\frac{2\pi}{\omega}} \int\limits_{-\infty}^{\infty} (\boldsymbol{\eta}) e^{i\omega t - i\omega \frac{\boldsymbol{n}}{c} t} dt$$

где η-единичный вектор поляризации кванта, $\boldsymbol{n}$-единичный вектор $\frac{k}{k}$.

Так как время соударения электрона много меньше, чем интервал t, существенный в этом интеграле, $t \sim \frac{1}{\omega\left(1 - \frac{vn}{c}\right)}$,

то можно считать, что скорость частицы в момент времени $t = 0$ скачкообразно изменилась с $v = v_1$ на $v = v_2$. Тогда из (1.41) находим

$$C_1 = i\sqrt{\frac{2\pi}{\omega}} \left\{ (v\eta) \left. \frac{e^{i\omega\left(t - \frac{vn}{c} t\right)}}{i\omega\left(1 - \frac{vn}{c}\right)} \right|_{-\infty}^{0} + (v\eta) \left. \frac{e^{i\omega\left(t - \frac{vn}{c} t\right)}}{i\omega\left(1 - \frac{vn}{c}\right)} \right|_{0}^{\infty} \right\} =$$

$$= \sqrt{\frac{2\pi}{\omega^3}} \eta \left(\frac{v_1}{1 - \frac{v_1 n}{c} - \frac{v_2}{1 - \frac{v_2 n}{c}}} \right).$$

Для малых углов отклонения электрона и кванта из (1.42) получаем

$$C_1^2 \sim \frac{1}{\omega^3} \frac{(\Delta v)^2}{(1 - v/c)^2}$$

здесь Δv - изменение скорости электрона. Так как знаменатели выражения (1.42) при малых углах отклонения кванта ϑ_κ и электрона ϑ_e имеют вид

$$1 - \frac{v}{c} + \frac{(\vartheta_\mathrm{k} + \vartheta_\mathrm{e})^2}{2}, \quad 1 - \frac{v}{c} + \frac{\vartheta_\mathrm{K}^2}{2},$$

то существенные углы отклонения ограничены условием

$$\boldsymbol{\vartheta}_\mathrm{k}, \boldsymbol{\vartheta}_\mathrm{e} \leqslant \sqrt{1 - \frac{v}{c}}.$$

Оценим вероятность испускания кванта в интервал частот $[\omega, \omega + d\omega]$ при заданном изменении скорости электрона Δv. Для этого умножим (1.43) на статистический вес конечных состояний кванта $dk/(2\pi)^3$:

$$dW \sim \frac{1}{\omega^3} \frac{(\Delta v)^2}{\left(1 - \frac{v}{c}\right)^2} k^2 dk d\Omega_{\mathrm{K}} \sim \frac{(\Delta v)^2}{c^3 \left(1 - \frac{v}{c}\right)^2} \frac{d\omega}{\omega} \vartheta_{\mathrm{K}} d\vartheta_{\mathrm{K}}.$$

Сечение тормозного излучения равно произведению вероятности испускания кванта dW на сечение кулоновского рассеяния для релятивистских электронов:

$$d\sigma_{\mathrm{T,h}} \sim \frac{(\Delta v)^2 \vartheta_{\mathrm{K}}^2}{c^3 \left(1 - \frac{v}{c}\right)^2} \frac{d\omega}{\omega} \cdot \frac{Z^2}{E^2} \frac{d\Omega_{\mathrm{e}}}{\sin^4 \frac{\theta_{\mathrm{e}}}{2}}$$

или при малых углах рассеяния ($\sin \theta_{\mathrm{e}} \approx \theta_{\mathrm{e}} \approx q/p$)

$$d\sigma_{T,u} \sim \frac{q^2 \left(1 - \frac{v}{c}\right)}{c^3 \left(1 - \frac{v}{c}\right)} \frac{d\omega}{\omega} \cdot \frac{Z^2}{p^2 c^2} \frac{\theta_{\mathrm{e}} d\theta_{\mathrm{e}}}{\theta_{\mathrm{e}}^4} \sim \frac{Z^2}{c^5} \frac{d\omega}{\omega} \frac{dq}{q}.$$

Найдем вероятность иснускания кванта для произвольного изменения импульса электрона. Для этого проинтегрируем (1.46) по q. Будем считать электрон ультрарелятивистским, т. е. $1 - v/c \ll 1$. Так как $Ze^2; \hbar c \ll 1$, то минимальный угол отклонения будет определяться дифракцией электрона на радиусе атома $a \sim Z^{-1/3}$, а максимальный условием (1.44).

Мнтегрируя (1.46) по q, получаем

$$\int \frac{d\sigma_{\text{Т. и}}}{dq} dq \sim \frac{Z^2}{c^5} \frac{d\omega}{\omega} \ln \frac{q_{\max}}{q_{\min}} \sim \frac{Z^2}{c^5} \frac{d\omega}{\omega} \ln \frac{c}{Z^{1/3}}.$$

Оценим сечение тормозного излучения квантов с произвольными частотами. Интегрируя (1.47) по ω, находим

$$\sigma_{\text{т.и}} \sim \frac{Z^2}{c^5} \ln \frac{c}{Z^{1/3}} \cdot \ln \frac{\omega_{\max}}{\omega_{\min}}.$$

Максимальная частота кванта - порядка энергии электрона:

$$\omega_{\max} \sim \frac{mc^2}{\sqrt{1 - v^2/c^2}}.$$

При $\omega_{\min} \to 0$ выражение (1.48) расходится (см. стр. 109). Однако потери энергии электрона на тормозное излучение будут конечными: $-\frac{dE}{dx} = \int N \omega d\sigma$ и, где N число ядер в единице объема. Окончательно,

$$-\frac{dE}{dx} \sim \frac{Z^2 N}{c^5} E \ln \frac{c}{Z^{1/3}}$$

13.2.5 Pair Production (!!!)

Напомним читателю, что релятивистски инвариантное уравнение диижения электрона - уравнение Дирака - при заданном импульсе p электрона имеет собственные функции, отвечающие не только положительным, но и отрицательным значениям энергии: $E = \pm\sqrt{m^2c^4 + p^2c^2}$. Для того чтобы объяснить, почему электрон не переходит в отрицательные состояния с испусканием кванта, Дирак предположил, что все отрицательные состояния в вакууме заполнены электронами. Тогда переход в эти

состояния запрещен принципом Паули. Незаполненное отрицательное состояние означает, что в вакууме есть позитрон.

С этой точки зрения механизм образования пар аналогичен механизму фотоэффекта: квант переводит электрон из состояния с отрицательной энергией в состояние с положительной энергией. В пустоте такой процесс невозможен, как это сразу видно из законов сохранения энергии и импульса. В поле ядра процесс делается возможным, так как электрон передает излишек импульса ядру.

Можно оценить сечение образования пар на ядре аналогично тому, как это делалось для тормозного излучения: найти вероятность образования пар при заданной величине передаваемого ядру импульса, а затем умножить эту вероятность на сечение рассеяния электрона на ядре и проинтегрировать по всем значениям передаваемого импульса.

Можно получить сечение образования пар, рассматривая этот процесс как обратный тормозному излучению. Строго говоря, процесс, обратный тормозному излучениіо, соответствует поглощеиию кванта и переходу электрона из одного состояния с положительной энергией в другое. Однако в ультрарелятивистском случае, которым мы для простоты ограничимся, собственные функции, соответствующие отрицательной энергии (т. е. соответствующис позитрону), мало отличаются от функций для положительной энергии (кулоновское поле ялра вносит малую поправку). Следовательно, сечение образования пар можно приближенно рассматривать как процесс, обратный тормозному излучению.

Сечения прямого и обратного процессов относятся как статистические веса конечных состояний. В случае тормозного излучения в конечном состоянии есть электрон и квант, тогда как в случае образования пар-позитрон и электрон. Но при больиих энергиях статистический вес кванта не отличается от статистического веса электрона той же энергии, и поэтому сечение образования пар совпадает по порядку величины с сечением тормозного излучения, проинтегрированным по энергиям квантов порядка энергии электрона. Таким образом,

$$\sigma_{\text{пар}} \sim \frac{Z^2}{c^5} \ln \frac{c}{Z^{1/3}}.$$

Потери энергии квантов на единице пути вследствие образования пар имеют порядок

$$-\frac{dE}{dx} \sim \frac{NZ^2}{c^5} E \ln \frac{c}{Z^{1/3}},$$

т. е. совпадают по порядку величины с потерями энергин ультрарелятивистского электрона на тормозное излучение.

13.2.6 Lamb Shift

Электрон атома, взаимодействуя с нулевыми колебаниями электромагнитного поля, дрожит на своси орбите. Вследствие этого его заряд размазывается в пространстве и взаимодействие с кулоновским полем ядра ослабевает. Такнм образом, уровни энергии из-за взаимодействия с нулевыми колебаниями повышаются. Это явление называется лэмбовским смещением. Оценим величину смещения.

Пусть δ-отклонение электрона от равновесного положения из-за взаимодействия с нулевыми колебаниями. Тогда изменение потенциала взаимодействия равно

$$H' = V(r+\delta) - V(r) = \frac{\partial V}{\partial r}\delta + \frac{1}{2}\frac{\partial^2 V}{\partial x_i \partial x_j}\delta_i \delta_j (i,j = x,y,z),$$

Здесь $\boldsymbol{r}$-координата электрона относительно ядра. Усредним это выражение по дрожанию электрона. Тогда $\overline{\delta} = 0$, а $\overline{\delta_x^2} = \overline{\delta_y^2} = \overline{\delta_z^2} = \frac{1}{3}\overline{\delta^2}$. Следовательно,

$$H' = \frac{1}{6}\overline{\delta^2}\Delta V.$$

Итак, для определения величины лэмбовского смещения необходимо знать средний квадрат амплитуды дрожания электрона $\overline{\delta^2}$.

Уравиение движения электрона в поле нулевых колебаний E для оценок можно записать в виде

$$-\ddot{\boldsymbol{\delta}} = +E + \omega_{\text{ar}}^2\delta,$$

где ω_{ax} - частота обращения электрона. Предположим, что частота дрожания электрона много больше $\omega_{\text{ат}}$. Тогда членом $\omega_{a\tau}^2\delta$ в этом выражении можно пренебречь.

Разложим в ряд Фурье отклонение электрона δ и поле нулевых колебаний E:

$$\delta = \sum_{k\lambda}\delta_{k\lambda}e^{-i\omega_{k\lambda}^t}, \quad E = \sum_{k\lambda}E_{k\lambda}e^{-i\omega_{\text{mot}}^*}$$

При этом мы предположили, что $k\delta \ll 1$. Ниже мы в этом убедимся.

Уравнение движения электрона в фурье-представлении приобретает вид

$$\omega_{k\lambda}^2\delta_{k\lambda} = E_{k\lambda}.$$

Средний квадрат амплитуды дрожания $\overline{\delta^2}$ равен

$$\overline{\delta^2} = \sum_{k\lambda}\bar{\delta}_{k\lambda}^2 = \sum_{k\lambda}\frac{E_{k\lambda}^2}{\omega_{k\lambda}^4}.$$

Найдем $E_{k\lambda}^2$. Энергия нулевых колебаний типа $k\lambda$ равна

$$\delta_{k\lambda} = \int\frac{E_{k\lambda}^2}{4\pi}dV = \frac{E_{k\lambda}^2}{4\pi} = \frac{1}{2}\omega_{k\lambda}$$

(нормировочный объем равен 1). Отсюда $E_{k\lambda}^2 = 2\pi\omega_{k\lambda}$; следовательно,

$$\overline{\delta^2} = 2\pi\sum_{k\lambda}\frac{1}{\omega_{k\lambda}^3}.$$

Заменим суммирование по k интегрированием:

$$\sum_{k\lambda} = 2\int\frac{4\pi k^2dk}{(2\pi)^3} = \frac{1}{\pi^2}\int\frac{\omega^2d\omega}{c^3}$$

(множитель 2 возникает из суммы по двум поляризациям кванта). Тогда получаем

$$\overline{\delta^2} = \frac{2}{\pi c^3}\int\frac{d\omega}{\omega} = \frac{2}{\pi c^3}\ln\frac{\omega_{\max}}{\omega_{\min}}.$$

Каковы пределы интегрирования в этом выражении? $\omega_{\max}$ определяется условием нерелятивистского движения электрона в поле нулевых колебаний. Действительно, если электрон при дрожании приобретает релятивистский импульс, то в уравнение движения войдет релятивистская масса и $\delta_{k\lambda}$ будет уменьшена. Поэтому интеграл обрезается условием $k \ll c, \omega \ll c^2$. При этом величина $k\delta$, которой мы пренебрегли, $k\delta \sim c^{-112} \ll 1$.

$\omega_{\mathbf{mn}}$ определяется из того условия, что, как мы предположили, частота поля должна быть не меньше, чем частота обращения электрона на атомной орбите ω_{ar}. Как легко видеть из уравнения для δ, область $\omega < \omega_a^{\text{вносит}}$ малый вклад. Итак, $\overline{\delta^2} = \frac{2}{\pi c^3}\ln\frac{\omega_{\max}}{\omega_{a\tau}}$.

Так как $\overline{\delta^2}$ логарифми- чески зависит от ω_{mln} и $\omega_{\max}$, то нетичноств в их определении несущественна.

Смещение электронного терма в первом поорядке теории возмущений дается днагональным матричным элементом возмущения H' по состоянию электрона Ψ_n, т. е.

$$\delta E = \frac{1}{6}\overline{\delta^2}\int \Psi_n \Delta V \Psi_n dr = \frac{1}{6}\overline{\delta^2}\int \Psi_n 4\pi\rho\Psi_n dr,$$

где ρ - плотность заряда. Так как заряд ядра сосредоточен в области, малой по сравнению с радиусом электронной орбиты, то электронную волновую функцию можно взять в начале координат. Интеграл $\int \rho dr$ равен заряду ядра Z.Итак,

$$\delta E = \frac{2\pi Z}{3}\overline{\delta^2}\left|\Psi_n(0)\right|^2 = \frac{4Z}{3c^3}\left|\Psi_n(0)\right|^2 \ln\frac{\omega_{\max}}{\omega_{\min}},$$

т. е. лэмбовское смещенне определяется значением волновой функции электрона в начале координат.

Таким образом, смещение имеет заметнуго величину лишь для s-электронов, так как только для них отсутствует центробежный барьер и электрон может находиться в начале координат. Смещение электронных термов, обладающих угловым моментом, будет значительно меньшим.

Лэмбовское смещение приводит к расщеилению термов $2s_{1/2}$ и $2p_{1,2}$ водородонодобного атома. Согласно сказанному выше уровень $2p_{1/2}$ смешается значительно слабее, чем $2s_{1/2}$. Так как $\left|\Psi_{2s}(0)\right|^2 = Z^3/8\pi$, то $\delta E = \frac{4Z}{3c^3}\frac{Z^3}{8\pi}\ln\frac{c^2}{Z^2} = \frac{Z^4}{6\pi c^3}\ln\frac{c^2}{Z^2}$

13.2.7 Divergence of Series in Quantum Electrodynamics

В квантовой электродинамике используют теорию возмучений по электромагнитному взаимодействию. Действительно, ряды теории возмущений содержат безразмерный малый параметр $e^2/\hbar c \approx 1/137$.

Покажем, что эти ряды асимптотические, т. е. расходятся при увеличении числа членов. Существует оптимальное число членов ряда, которое лучше всего изображает изучаемый процесс. Нже это число будет оценено. Для этого прежде всего убедимся, что физические величнны как функции e^2 имеют особую точку при $e^2 = 0$ и, следовательно, не могут быть разложены в ряд по степеням e^2.

В качестве примера рассмотрим энергию вакуума (Дайсон, 1952). Если бы не было особой точки при $e^2 = 0$, то энергня вакуума не зависела бы от способа стремления e^2 к нулю. Пусть энергия вакуума, найденная по теории возмушений, стремится к E_0. какой величине стремится энергия вакуума, когда $e^2 \longrightarrow 0$ со стороны отрицательных значений? Рассмотрим при $e^2 < 0$ рождение в вакууме N электронно-позитронных пар. ГПри $e^2 < 0$ электроны (так же как и позитроны) притягнваются друг к другу. Определим, при каком N процесс образования пар энергетически выгоден. Пусть электронное и позитронное облака разошлись на достаточно большое расстояние друг от друга, так что отталкиванием между ними можно пренебречь. Энергиь каждого из этих облаков можно оценить по методу Томаса Ферми. Находим, что выигрыш в энергии $-E \sim N^{\gamma/3}$. Проигрыш в энергии составляет $2mc^2$ на каждую электроннопозитронную пару, а для всех частиц $2mc^2N$. Следовательно, если $N^{7/3} > c^2N$, т. е. если $N > c^{3/2}$, то рождение электронно-позитронных пар оказывается выгодньм.

При $N \sim c^{3/2}$ величина $\varphi \sim c^2$, поэтому нужно рассмотреть, какой результат получится в релятивистском случае. Рассмотрим для простоты ультрарелятивистский предел. В этом случае $p_0 \sim \varphi/c$, следовательно (стр. 36), $\frac{\varphi}{l^2} \sim \left(\frac{\varphi}{c}\right)^3$, откуда $\varphi l \sim c^{3/2}$. Так как $N \sim \frac{\varphi}{l^2}l^3$, то получаем $N \sim \varphi l \sim c^{3/2}$, т. е. ту же оценку, что и в нерелятивистском случае.

Энергия системы при этом - $E \sim N\varphi \sim c^3/l$, т. е. может быть неограниченно понижена уменьцением L. Мы получили, что электромагнитный вакуум при $e^2 < 0$ оказывается неустойчивым. Так как при $e^2 > 0$ он устойчнв, то это означает, что имеется особая точка при $e^2 = 0$.

Рождение N электронно-позитронных пар соответствует N-му порядку теории возмущений. Найденное число $N \sim c^{z/2}$ указывает порядок числа членов теории возмущений, начиная с которого будет сказываться особая точка при $e^2 = 0$. Учет более высоких порядков теории возмущений не улуч шит, а ухудиит результат.

13.3 Light-Matter Interactions

(it is a big topic and there are many research about it. see cond matter for now about it, but I'll write here some important concepts)

14 Atomic and Nuclear Physics

14.1 Radiation, Transitions in Atoms

(!! write it later, this is a very important part of QM)

14.1.1 Typical radiation

(all what one needs to solve problems)

14.1.2 Taking into account special features in radiation

How lattice symmetries determine rules of radiation?

(answer to this question. Currently, I don't know)

14.2 Hydrogen atom with extra physics

14.2.1 Relativistic hydrogen atom

(потом допишу его)

14.2.2 Fine Splitting and Spin–Orbit Interaction

Классическое выражение энергии спин-орбитального взаимодействия

Пусть электрон движется равномерно и прямолинейно со скоростью v в поле ядра, помещённого в начале системы координат 1 и которое создаёт кулоновское поле $e\mathbf{E} = -\frac{\mathbf{r}}{r}\frac{\partial V}{\partial r}$. В системе координат 2, связанной с движущимся электроном, наблюдатель будет видеть движущееся ядро, которое создает как электрическое, так и магнитное поле, с напряженностью $'$ и $'$, соответственно. Как следует из теории относительности $\mathbf{E}'$ и $\mathbf{H}'$ связаны с $\mathbf{E}$ следующими соотношениями:

$$\mathbf{E}' = \mathbf{E}, \quad \mathbf{H}' \approx -\frac{1}{c}\mathbf{v} \times \mathbf{E} = -\frac{1}{mc}\mathbf{p} \times \mathbf{E}$$

Где отброшены члены порядка v^2/c^2. Тогда уравнение изменения спинового момента количества движения $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$ (связанного гиромагнитным отношением как $\frac{|\boldsymbol{\mu}|}{|\mathbf{S}|} = \frac{|e|}{mc}$) в системе координат 2 будет иметь вид:

$$\frac{d\mathbf{S}}{dt} = \mu \times \mathbf{H}' = -\frac{e\hbar}{2m^2c^2}\boldsymbol{\sigma} \times [\mathbf{p} \times \mathbf{E}].$$

Это уравнение соответствует взаимодействию спина электрона с электромагнитным полем, которое описывается гамильтонианом следующего вида:

$$\mathcal{H}'_{so} = \frac{e\hbar}{2m^2c^2}\boldsymbol{\sigma} \cdot \mathbf{p} \times \mathbf{E}.$$

Совпадение с другой формулой (!?!??!)

Заметим, что вид гамильтониана с точностью до множителя 1/2 совпадает с видом спин-орбитальной части гамильтониана полученного из уравнения Дирака с помощью преобразования Фолди и Ваутхайзена.

Отсутствие этого множителя связано с тем, что уравнение изменения магнитного момента электрона будет верно только в том случае, если система 2 не будет вращающейся, в противном случае это уравнение, из-за прецессии Томаса, должно иметь вид

$$\frac{d\mathbf{S}}{dt} = \frac{e\hbar}{2mc}\boldsymbol{\sigma} \times \mathbf{H}' - \omega_T \times \mathbf{S}$$

где ω_T - томосовская угловая скорость вращения. Электрон в атоме ускоряется экранированным кулоновским полем поэтому томосовская угловая скорость описывается соотношением

$$\omega_T \approx \frac{1}{2m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}[\mathbf{r} \times \mathbf{p}]$$

Таким образом гамильтониан спин-орбитального взаимодействия будет иметь вид:

$$\mathcal{H}_{so} = \frac{\hbar}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}\boldsymbol{\sigma} \cdot \mathbf{r} \times \mathbf{p} - \frac{\hbar}{4m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}\boldsymbol{\sigma} \cdot \mathbf{r} \times \mathbf{p} = \frac{\hbar}{4m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}\boldsymbol{\sigma} \cdot \mathbf{r} \times \mathbf{p}$$

Что в точности совпадает с ранее полученным результатом.

Связь спин орбитального взаимодействия с прецессией Томаса (??)

Об аналогии, что в системе электрона имеется поле от тока атома (??)

14.2.3 Stark Effect

теория эффекта Штарка

Гамильтониан атома водорода, помещённого в однородное электрическое поле, имеет вид

$$H = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{r} + e\mathcal{E}r\cos\vartheta \equiv H_0 + V$$

Волновая функция основного состояния атома водорода с гамильтонианом H_0 в координатном представлении

$$\psi_{(0)}(\mathbf{r}) = \langle \mathbf{r}|\psi_{(0)}\rangle = \frac{1}{\sqrt{\pi a^3}}e^{-\frac{r}{a}}$$

Поправка первого порядка ϵ_1 к энергии по теории возмущений равна нулю в силу сферической симметрии волновой функции основного состояния.

Действительно,

$$\epsilon_1 = \left\langle \psi_{(0)} | V | \psi_{(0)} \right\rangle = 2\pi e\mathcal{E} \int\limits_0^\infty dr \frac{r^3}{\pi a^3} e^{-\frac{2r}{a}} \int\limits_0^\pi \cos\vartheta \sin\vartheta d\vartheta = 0$$

Поправку к энергии второго порядка по теории возмущений можно вычислить через поправку первого порядка к волновой функции $\psi_{(1)}(\mathbf{r})$

$$\epsilon_2 = \left\langle \psi_{(0)} | V | \psi_{(1)} \right\rangle = e\mathcal{E} \int d_3x \psi_{(0)}(\mathbf{r}) \cdot r\cos\vartheta \cdot \psi_{(1)}(\mathbf{r})$$

Поправка первого порядка к волновой функции $\psi_{(1)}(\mathbf{r})$ с учётом (5.3) удовлетворяет уравнению

$$\left(-\frac{\hbar^2}{2m}\Delta - \frac{e^2}{r} + \frac{me^4}{2\hbar^2} \right) \psi_{(1)}(r,\vartheta) = -V\psi_{(0)}(\mathbf{r}) = -\frac{e\mathcal{E}r}{\sqrt{\pi a^3}} \cos\vartheta \cdot e^{-\frac{r}{a}}$$

Вспоминая, что лапласиан в сферических кооридинатах имеет вид

$$\triangle = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2}\Delta_{\vartheta,\varphi}, \quad \Delta_{\vartheta,\varphi} = \frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta \frac{\partial}{\partial\vartheta} \right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}$$

будем искать решение уравнения (5.5) в виде

$$\psi_{(1)}(r,\vartheta) = f(r) \cdot e^{-\frac{r}{a}} \cos\vartheta, \quad f(r) = a_0 + a_1 r + a_2 r^2.$$

Подставляя (5.6) в (5.5), получаем

$$\begin{gathered} -\tfrac{\hbar^2}{2m}\left[f''(r) + \tfrac{2}{r}f'(r) - \tfrac{2}{a}f'(r) - \tfrac{2}{ra}f(r) + \tfrac{1}{a^2}f(r) \right] e^{-\frac{r}{a}} \cos\vartheta + \tfrac{\hbar^2}{mr^2} f(r) \cdot e^{-\frac{r}{a}} \cos\vartheta - \\ -\tfrac{e^2}{r} f(r) \cdot e^{-\frac{r}{a}} \cos\vartheta + \tfrac{me^4}{2\hbar^2} f(r) \cdot e^{-\frac{r}{a}} \cos\vartheta = -\tfrac{e\mathcal{E}r}{\sqrt{\pi a^3}} \cos\vartheta \cdot e^{-\frac{r}{a}} \end{gathered}$$

Расписывая функцию $f(r)$ и её производные, имеем

$$-\frac{\hbar^2}{m}\left[3a_2 + \frac{a_1}{r} - \frac{2a_1}{a} - \frac{3a_2}{a}r - \frac{a_0}{ar} \right] + \frac{\hbar^2}{mr^2} f(r) - \frac{e^2}{r} f(r) + \left[\frac{me^4}{2\hbar^2} - \frac{\hbar^2}{2ma^2} \right] f(r) = -\frac{e\mathcal{E}r}{\sqrt{\pi a^3}}$$

что после тождественных преобразований даёт

$$\frac{\hbar^2}{m}\left[\frac{a_0}{r^2} - 2a_2 + \frac{2a_1}{a} + \frac{3a_2}{a}r \right] - e^2\left(a_1 + a_2 r \right) = -\frac{e\mathcal{E}r}{\sqrt{\pi a^3}}$$

Из последнего выражения находим, что

$$a_0 = 0, \quad a_1 = -a\frac{\mathcal{E}}{e\sqrt{\pi a^3}}, \quad a_2 = -\frac{\mathcal{E}}{2e\sqrt{\pi a^3}}$$

Подставляя полученные коэффициенты в функцию $f(r)$, находим

$$\psi_{(1)}(r,\vartheta) = f(r) \cdot e^{-\frac{r}{a}} \cos\vartheta = -a\frac{\mathcal{E}r}{e\sqrt{\pi a^3}}\left(1 + \frac{r}{2a} \right) \cdot e^{-\frac{r}{a}} \cos\vartheta.$$

С учётом (5.9) уравнение (5.4) для поправки к энергии во втором порядке теории возмущений принимает вид

$$\epsilon_2 = e\mathcal{E} \int d_3x \psi_{(0)}(\mathbf{r}) \cdot r\cos\vartheta \cdot \psi_{(1)}(\mathbf{r}) = -2\pi\frac{\mathcal{E}^2}{\pi a^2} \int\limits_0^\infty dr r^4 \left(1 + \frac{r}{2a} \right) \cdot e^{-\frac{2r}{a}} \int\limits_0^\pi \cos^2\vartheta d\vartheta$$

Или

$$\epsilon_2 = -\frac{4}{3}\frac{\mathcal{E}^2}{a^2}\int\limits_0^\infty drr^4\left(1+\frac{r}{2a}\right)\cdot e^{-\frac{2r}{a}} = -\frac{4}{3}\mathcal{E}^2a^3\int\limits_0^\infty dxx^4\left(1+\frac{x}{2}\right)\cdot e^{-2x}$$

Интеграл

$$I = \int\limits_0^\infty dxx^4\left(1+\frac{x}{2}\right)\cdot e^{-2x} = \frac{27}{16}$$

и поэтому

$$\epsilon_2 = -\frac{9}{4}\mathcal{E}^2a^3 = -\frac{9}{4}\frac{\hbar^6\mathcal{E}^2}{m^3e^6}$$

Из выражения (5.11) находим поляризуемость κ атома по формуле

$$\kappa = -\frac{\partial^2\epsilon_2}{\partial\mathcal{E}^2} = \frac{9}{2}a^3 = \frac{9}{2}\frac{\hbar^6}{m^3e^6}$$

Применения эффекта Штарка

(?? почитаю книги для экспериментаторов)

14.2.4 Zeeman effects: basics

Эффект Зеемана по общей физике

Эффект Зеемана в слабых магнитных полях??

Основные формулы (??)

общефизическое представление

Прежде всего обратимся к влиянию внутренних полей.

Со спиновым механическим моментом электрона s связан магнитный момент

$$\mu_{\rm s} = -\frac{e}{m}\,{\rm s}$$

Это означает, что при наличии магнитного поля произойдет взаимодействие спина с последним, и появится дополнительная «магнитная» энергия.

На примере атома водорода мы видели,

что существование магнитного момента электрона приводит к появлению спин-орбитального взаимодействия, в результате которого уровни с $l \neq 0$ расщепляются по энергии на два подуровня с $j = l \pm 1/2$ -как говорят, возникает тонкая структура уровней.

Такое расщепление мало по сравнению с расстоянием между уровнями с разными n (см. формулу (6.54)).

Сразу отметим, что энергия спин-орбитального взаимодействия, а значит и величина расщепления, зависят от l; это хорошо видно из той же формулы (6.54)

На рис. 8.2 приведен пример тонкой структуры водородоподобного атома с $n = 2$: уровень с $l = 1$ расщеплен на два с$j = l \pm s = l \pm 1/2$, спектроскопические обозначения которых $P_{3/2}$ и $P_{1/2}$.

Спин-орбитальное взаимодействие снимает вырождение уровней по l (вспомним, что в чисто кулоновском поле энергия зависит только от $n, 0 \leqslant l \leqslant n-1$, с каждым l связано $(2l+$

1) -кратное вырождение по m_l, итого с учетом спина получается $2n^2$ -кратное вырождение или $2n^2$ -мультиплетность уров ня).

Мы уже упоминали хорошо известный пример снятия такого вырождения у натрия, в спектре которого наблюдается желтый дублет с длинами волн 5890 и 5896 Å.

Аналогично, взаимодействие магнитного момента ядра со спиновыми и орбитальными магнитными моментами электронов приводит к появлению сверхтонкой структуры атомных спектров.

Интервалы этого расщепления чрезвычайно малы: их масштаб на два-три порядка меньше масштаба расщепления, обусловленного тонкой структурой.

Поэтому сверхтонкая структура может рассматриваться для каждой из компонент тонкой структуры в отдельности.

Если спин ядра обозначить через I, а электронной оболочки - через J, то полный момент атома будет равен $\mathbf{F} = \mathbf{J} + \mathbf{I}$, и F пробегает значения

$$F = J + I, J + I - 1, ..., |J - I|$$

Соответственно, число компонент сверхтонкой структуры уровня с данным J равно $2I+1$(если $J > I$) или $2J + 1$(если $J < I$). Перейдем теперь к рассмотрению поведения атома во внешнем магнитном поле - эффекту Зеемана.

Это явление - расщепление спектральных линий в магнитном поле - было открыто голландским физиком П. Зееманом в 1896 г.

С внешним магнитным полем взаимодействуют как орбитальный, так и спиновый магнитные моменты электронов.

Кроме того, нужно иметь в виду, что эти магнитные моменты взаимодействуют между собой (знакомое нам спин-орбитальное взаимодействие).

В зависимости от относительной величины указанных взаимодействий различают два случая: слабого магнитного поля и сильного магнитного поля.

В первом случае взаимодействие внешнего магнитного поля с орбитальным и спиновым магнитными моментами электронов существенно меньше спин-орбитального взаимодействия, и в результате расщепление уровней за счет внешнего магнитного поля оказывается меньшим, чем расщепление, обусловленное внутренним полем самого атома (тонкая структура).

Этот случай носит название сложного эффекта Зеемана, поскольку в сильных полях структура спектра оказывается намного проще (как мы увидим чуть позже).

Дополнительная энергия в магнитном поле в данном случае равна

$$E_B = -(\mu \mathrm{B}) = g\mu(\mathrm{JB}) = g\mu m_J B$$

Здесь m_J определяет проекции вектора $\mathbf{J}$ на направление внешнего поля B и принимает $2J + 1$ значений, т. е. все зависит от взаимной ориентации векторов J и B.

Расщепление уровней оказывается эквидистантным, а сама величина расщепления линейно растет с полем.

О таком случае говорят, что магнитное поле снимает вырождение уровней по m_J. Поскольку внешнее расщепление меньше внутреннего (тонкой структуры), то картина слегка расщепленных спектральных уровней остается практически такой же, как и без поля.

Хотя расщепление одного уровня является эквидистантным, значения фактора Ланде g, вообще говоря, различны у разных уровней, что приводит к возникновению сложного расщепления линий перехода.

При этом существенное значение имеют правила отбора для излучения.

Общефизное описание расщепление линий натрия (??)

Классический пример эффекта Зеемана - поведение желтого дублета натрия в магнитном поле (сам дублет есть проявление тонкой структуры уровней).

Основное состояние натрия $3^2S_{1/2}$, а выше расположены два возбужденных состояния $3^2P_{1/2}$ и $3^2P_{3/2}$.

На рис. 8.3 стрелками показаны переходы, разрешенные правилами отбора, запрещенные переходы показаны штриховыми линиями. В чисто кулоновском поле энергия зависит только от квантового числа n и поэтому, казалось бы, не должно быть разницы в энергии уровней с разными l. Однако реально это справедливо лишь для водорода и водородоподобных атомов, а в натрии внутренние электроны экранируют поле ядра, таким образом, для p-электронов заряд ядра как бы меньше, чем для s -электронов, и они располагаются несколько выше.

Из-за спин-орбитального взаимодействия p -уровень расщепляется на два (тонкая структура), и в спектре излучения появляется желтый дублет.

Величина спин-орбитального расщепления у натрия равна $U_{L_S} = 2 \times \times 10^{-3}$ эВ, а во внешнем поле $B = 10^2$ Тл оно, согласно формуле (8.11), порядка

$$\Delta U_B = \mu_0 \mu_{\text{B}} B = 4\pi \cdot 10^{-7} \cdot 9,3 \cdot 10^{-24} \cdot \left(10^6/4\pi\right) = \\ = 10^{-24}\text{Дж} \ = 6 \cdot 10^{-6} \ni \text{В} \ll U_{LS},$$

т. е. поля такого порядка являются слабыми.

Во внешнем поле уровень $3^2P_{1/2}$ расщепляется, как и уровень $3^2S_{1/2}$, на два подуровня с проекциями $m_J = \pm 1/2$, а уровень $3^2P_{3/2}$ - на 4 подуровня с $m_J = 3/2, 1/2, -1/2, -3/2$ (при этом уровень с $m_J = 3/2$ расположен выше всех, а с $m_J = -3/2$ - самый низкий, что непосредственно следует из формулы (8.11)).

Всего в слабом магнитном поле наблюдается 10 переходов.

В силу правил отбора ($\Delta m_S = 0,\ \Delta m_L = 0, \pm 1,\ \Delta m_J = 0, \pm 1$) подавлены переходы с $m_J = 3/2$ на уровень $m_J = -1/2$ и с$m_J = -3/2$ на $m_J = 1/2$. Еще раз подчеркнем: так много линий наблюдается из-за того, что у разных уровней разная величина расщепления.

Поэтому, в частности, переходы с уровня $3^2P_{1/2}$ на $3^2S_{1/2}$ между подуровнями с $(1/2 \to 1/2)$ и $(-1/2 \to -1/2)$ по энергии неравны.

Действительно, у всех рассмотренных нами уровней натрия значения фактора Ланде разные:

$$g_{\text{л}}\ \left(P_{3/2}\right) = 1 + \frac{3/2 \cdot 5/2 + 1/2 \cdot 3/2 - 1 \cdot 2}{2 \cdot 3/2 \cdot 5/2} = \frac{4}{3}$$

$$g_{\text{л}}\ \left(P_{1/2}\right) = 1 + \frac{1/2 \cdot 3/2 + 1/2 \cdot 3/2 - 1 \cdot 2}{2 \cdot 1/2 \cdot 3/2} = \frac{2}{3}$$

$$g_{\text{л}}\ \left(S_{1/2}\right) = 1 + \frac{1/2 \cdot 3/2 + 1/2 \cdot 3/2 - 0}{2 \cdot 3/2 \cdot 5/2} = 2$$

Простой эффект Зеемана в сильном поле

Теперь рассмотрим простой эффект Зеемана, наблюдаемый в сильном магнитном поле.

Здесь термин «сильное поле» означает, что энергия спин-орбитального взаимодействия U_{SL} намного меньше, чем энергия взаимодействия как спинового, так и орбитального магнитных моментов с внешним полем, т. е. $U_{SL} \ll U_{SB}, U_{LB}$. В случае слабого поля мы классифицировали состояния точно так же, как и без поля, а в данном случае этого делать уже нельзя.

Теперь мы считаем величину U_{SL} практически равной нулю, т. е. пренебрегаем данным взаимодействием.

Последнее означает, что оператор энергии не зависит от ориентации спинового и орбитального моментов, а следовательно, он не зависит и от суммарного вектора $\mathbf{J} = \mathbf{L} + \mathbf{S}$. Остается зависимость энергии лишь от проекций векторов $\mathbf{L}$ и $\mathbf{S}$ на вектор B, т. е. только от квантовых чисел m_L и m_S. Для этого случая существует жаргонное выражение: говорят, что в сильном поле «разрывается LS-связь».

Итак, учитывая, что $g_L = 1, g_S = 2$, магнитная часть энергии в сильном поле равна

$$U_B = g_L \mu m_L B + g_S \mu_e m_S B = \mu B$$

Теперь уже «нет» спин-орбитального расщепления, уровень 3^2P расщепляется на 5 компонент с $m_L + 2m_S = 2, 1, 0, -1, -2$, уровень 3^2S - на 2, как это показано на рис. 8.4.

В сильном поле 3 линии

Покажем, что в сильном поле всегда будут наблюдаться лишь 3 линии.

Пусть имеется два уровня с энергиями E_{01} и E_{02}, характеризующихся квантовыми числами $L1, L2, S1, S2$. Разность энергий этих уровней в сильном поле равна

$$\Delta U_B = [E_{02} + \mu B\,(m_{L2} + 2m_{S2})] - [E_{01} + \mu B\,(m_{L1} + 2m_{S1})]$$

Так как по правилам отбора возможны переходы только между уровнями с $m_{S1} = m_{S2}$, то

$$\Delta U_B = (E_{02} - E_{01}) + \mu B\,(m_{L2} - m_{L1})$$

Но $\Delta m_L = 0, \pm 1$, а значит, в спектрах излучения в сильном поле всегда будут наблюдаться лишь три линии - одна несмещенная и две смещенные на $\pm\mu B$. Вот почему эффект Зеемана в сильном магнитном поле называется простым.

В заключение рассмотрим, как будет поляризован свет при простом эффекте Зеемана.

Когда наблюдение ведется вдоль приложенного магнитного поля, эффект Зеемана называют продольным.

При этом, поскольку $\Delta m_S = 0$, а $\Delta m_L = 0, \pm 1$, уносимый фотоном момент равен 1 (дипольное излучение), и оказывается, что смещенные компоненты имеют круговую поляризацию (у них $\Delta m_L = \pm 1$).

Несмещенная компонента вообще видна не будет, так как для нее $\Delta m_L = 0$, а фотона с $m_z = 0$ не существует.

В поперечном эффекте Зеемана (наблюдение поперек магнитного поля) несмещенная линия - это просто линейно-поляризованный свет, а циркулярно поляризованные смещенные линии также будут выглядить как линейно-поляризованные волны

В результате при наблюдении в перпендикулярном направлении мы увидим три линейно-поляризованных волны.

Таким образом, энергетические уровни частиц (любых - это могут быть и ядра, и молекулы), обладающих ненулевыми магнитными моментами, во внешнем магнитном поле испытывают зеемановское расщепление.

Если облучать такие частицы внешним электромагнитным излучением с частотой, равной энергии переходов между подуровнями:

$$\omega = \frac{g \mu_\text{Ь} B}{\hbar}$$

то будет происходить резонансное поглощение излучения.

В зависимости от сорта частиц это может быть ЭПР - электронный парамагнитный резонанс, либо ЯМР - ядерный магнитный резонанс.

В последнем случае масштаб измерения магнитных моментов определяется не магнетоном Бора, а так называемым ядерным магнетоном $\mu_я = e\hbar/2m_p$, где m_p - масса протона, т.е. ядерный магнетон примерно в 1800 раз меньше магнетона Бора: он равен $5,05 \cdot 10^{-27}$ Дж/Тл $= 5,05 \cdot 10^{-24}$ эрг/Гс.

Обычно опыты проводят так, что частота генератора, создающего переменное электромагнитное поле, держится постоянной, а меняется внешнее магнитное поле B.

В образце энергия атомов с $\mu \neq 0$ зависит от ориентации магнитных моментов.

Если приложено внешнее поле, то после установления теплового равновесия в соответствии с больцмановским распределением заселенности уровней число частиц с моментами, ориентированными вдоль поля, оказывается больше числа частиц с противоположной ориентацией магнитных моментов.

Таким образом, результирующий магнитный момент образца становится отличным от нуля, т.е. образец намагничивается.

Этот эффект получил название парамагнитный резонанс, его впервые наблюдал советский физик Е.К. Завойский в 1944 г.

нормальное описание

как релятивистские поправки потом пропишу

Эффекты в магнитном поле

Основные формулы (??)

Описание атома водорода в магнитном поле

Гамильтониан взаимодействия электронов атома с постоянным внешним магнитным полем $\mathcal{H}$ есть:

$$H = \sum_f \left\{ \frac{1}{2m} \left(\boldsymbol{p}_f - \frac{e}{c} \boldsymbol{A}\left(\boldsymbol{r}_f\right) \right)^2 + \left(\boldsymbol{\mu}_f \cdot \boldsymbol{\mathcal{H}}\right) \right\} + V$$

здесь вклад вектор-потенциала происходит за счет ковариантной производной, V -потенциал, включающий в себя как нерелятивистские вклады кулоновского взаимодействия электронов с ядром и попарно друг с другом, так и релятивистские поправки, зависящие от спина.

Магнитный момент электрона, обусловленный спином, согласно уравнению Дирака с $g = 2$

$$\boldsymbol{\mu} = g \frac{e\hbar}{2mc} \boldsymbol{s}$$

Калибровка обычно фиксируется так, чтобы

$$\mathcal{A}(r) = \frac{1}{2}(\mathcal{H} \times r)$$

откуда заключаем, что

$$\operatorname{div} \boldsymbol{A}(\boldsymbol{r}) = \frac{1}{2} \epsilon_{\alpha\beta\gamma} \partial_\alpha \mathcal{H}_\beta x_\gamma = \frac{1}{2} \epsilon_{\alpha\beta\gamma} \mathcal{H}_\beta \delta_{\alpha\gamma} = 0$$

Поэтому при возведении в квадрат обобщенного импульса

$$\left(p - \frac{e}{c} \mathcal{A}(r) \right)^2 = p^2 - \frac{e}{c} \{ (p \cdot \mathcal{A}) + (\mathcal{A} \cdot p) \} + \frac{e^2}{c^2} \mathcal{A}^2$$

вклад ниже равен

$$(\boldsymbol{p}\cdot\boldsymbol{\mathcal{A}})+(\boldsymbol{\mathcal{A}}\cdot\boldsymbol{p})=2(\boldsymbol{\mathcal{A}}\cdot\boldsymbol{p})-\mathrm{i}\hbar\,\mathrm{div}\,\boldsymbol{\mathcal{A}}=\epsilon_{\alpha\beta\gamma}H_\alpha x_\beta p_\gamma=\mathcal{H}\cdot(\boldsymbol{r}\times\boldsymbol{p})=\hbar\boldsymbol{\mathcal{H}}\cdot\boldsymbol{l}$$

т.е. возникает член взаимодействия с магнитным моментом вращения:

$$\frac{1}{2m}\left(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A}(\boldsymbol{r})\right)^2=\frac{\boldsymbol{p}^2}{2m}-\frac{e\hbar}{2mc}(\boldsymbol{\mathcal{H}}\cdot\boldsymbol{l})+\frac{e^2}{8mc^2}(\mathcal{H}\times\boldsymbol{r})^2$$

Значит, гамильтониан атома в постоянном внешнем магнитном поле принимает вид

$$H=H_0^{\mathrm{at}}+\sum_f\left\{\mu_0\mathcal{H}\cdot(l_f+2s_f)+\frac{e^2}{8mc^2}\left(\mathcal{H}\times r_f\right)^2\right\}$$

где H_0^{at} - гамильтониан атома в отсутствие внешних источников, а магнетон Бора $\mu_0=e\hbar/2mc$. Суммирование орбитального момента и спина очевидно приводит к возмущению в Виде вза имодействия магнитного поля с магнитным моментом электронов атома:

$$V_{\text{mag.}}=\mu_0\mathcal{H}\cdot(\boldsymbol{L}+2\boldsymbol{S})$$

а квадратичный по полно член равен

$$V_d=\frac{e^2}{8mc^2}\sum_f\left(\mathcal{H}\times r_f\right)^2=\frac{e^2\mathcal{H}^2}{8mc^2}\sum_f r_f^2\sin^2\theta_f.$$

Он обусловливает диамагнитные свойства электронов, потому что коэффициент при квадрате поля имеет положительный знак: наведенный магнитный момент пропорционален внешнему полю $\boldsymbol{\mu}_{\text{ext.}}=B\mathcal{H}$, и он дает вклад в потенциальную энергию $U_{\text{ext.}}=-(\boldsymbol{\mu}_{\text{ext.}}\cdot\mathcal{H})$ так что, если $B<0$, то наведенный магнитный момент направлен против внешнего поля и положительна.

Количественная оценка

Оценим по порядку величины вклад во взаимодействие магнитного момента электронов и диамагнитный член.

Для этого прежде введем напряженность поля, характерную для атома:

$$\mathcal{H}_{\mathrm{at}}=\frac{e}{a^2}\sim 2\cdot 10^7\ \text{Гаусс.}$$

тогда

$$\mu_0\mathcal{H}\sim\frac{e^2\hbar}{mca^2}\frac{\mathcal{H}}{\mathcal{H}_{\mathrm{at}}}=\frac{e^2}{\hbar c}\frac{\hbar^2}{ma^2}\frac{\mathcal{H}}{\mathcal{H}_{\mathrm{at}}}=mc^2\alpha_{\mathrm{em}}^3\frac{\mathcal{H}}{\mathcal{H}_{\mathrm{at}}}$$

и, если $L\neq 0$ или $S\neq 0$, энергия взаимодействия магнитного момента с постоянным магнитным полем при $\mathcal{H}\ll\alpha_{\mathrm{em}}\mathcal{H}_{\mathrm{at}}\sim 10^5$ Гс оказывается существенно меньше энергии спин-орбитального взаимодействия за счет релятивистских поправок.

Диамагнитный вклад:

$$V_d\sim\frac{e^2}{mc^2}a^2\frac{e^2}{a^4}\frac{\mathcal{H}^2}{\mathcal{H}_{\mathrm{at}}^2}=\frac{e^4}{\hbar^2c^2}\frac{\hbar^2}{ma^2}\frac{\mathcal{H}^2}{\mathcal{H}_{\mathrm{at}}^2}=mc^2\alpha_{\mathrm{em}}^4\frac{\mathcal{H}^2}{\mathcal{H}_{\mathrm{at}}^2}$$

Отсюда немедленно следует, что если магнитный момент электронов не равен тождественно нулю, то диамагнитным вкладом заведомо можно пренебречь, поскольку он сравнивается с членом магнитного момента только при гигантских полях порядка

$$\mathcal{H}\sim\frac{\mathcal{H}_{\mathrm{at}}}{\alpha_{\mathrm{em}}}\sim 10^9\ \text{Гс}$$

При которых и поправки за счет магнитного момента становятся сравнимыми с энергией связи в атоме, т.е. поля становятся настолько велики, что приводят к ионизации атома,

Аномальный эффект Зеемана (??)

Основные формулы (??)

Если поместить излучающее тело в магнитное поле, за счет *эффекта Зеемана* спектр линий расщепится и появятся еще (?) две компоненты.
(???)

модель аномального эффекта Зеемана

(что это? где связь с эл?) магнитный диполь имеет энергию $U = -\vec{\mu}\vec{H}$.
черт, нужно в магнитном моменте разбираться!!! (потом доучу это все)
итак, магнитный момент (?????) $\vec{\mu} = \frac{e}{2c}[h, \vec{v}] = \frac{e}{2mc}[h, \vec{p}] = \frac{e}{2mc}\vec{L}$
в итоге энергия $U = -\frac{e}{2mc}\vec{L}\vec{H}$.
Если магнитный момент терма не равен нулю, То взаимодействие атома со слабым внешним Магнитным полем $\mathcal{H} \ll \alpha_{\rm em}\mathcal{H}_{\rm at} \sim 10^5$Гс является малым возмущением по сравнению с релятивистски ми спин-орбитальным и поправками.

Это означает, что в качестве волновых функций ведущего приближения следует рассматривать термы $^{2S+1}L_J$ В возмущении (10.5) магнитное поле задает выделенное направление, которое примем За направление оси z. Коммутатор

$$[J_\alpha, (\mathcal{H} \cdot \{\boldsymbol{J} + \boldsymbol{S}\})] = \mathrm{i}\epsilon_{\alpha\beta\gamma}\mathcal{H}_\beta\{J + S\}_\gamma$$

обращается в нуль для J_z. Далее, используя алгебру коммутаторов для произведения, легко Найти, ЧТО

$$\left[\boldsymbol{J}^2, (\mathcal{H} \cdot \{\boldsymbol{J} + \boldsymbol{S}\})\right] = 0$$

дение по M_J, которое имело место в отсутствие магнитного поля вследствие того, что сохранялись и компоненты $J_\pm : [J_\pm, H_0^{\rm at}] = 0$, некоммутирующе с$J_z : [J_\pm, J_z] \neq 0$, теперь ОКазывается "снятым": энергия зависит от M_J.

Для Вычисления матричного элемента возмущения заметим, что операторы полного момента и спина являются неприводимыми тензорными операторами первого порядка, Т.е. момента 1, так как при вращениях они преобразуются соответствующим образом - как векторы.

Отсюда следует, во-первых, элементарно

$$\langle J, M_J \,|J_z|\, J, M'_J\rangle = M_J\delta_{M_JM'_J}$$

Для вычисления матричного элемента возмущения заметим, что операторы полного момента и спина являются неприводимыми тензорными операторами первого порядка, Т.е. момента 1, так как при вращениях они преобразуются соответствующим образом - как векторы.

Отсюда следует, во-первых, элементарно

$$\langle J, M_J \,|J_z|\, J, M'_J\rangle = M_J\delta_{M_JM'_J}$$

а во-вторых,

$$[J_z, S_z] = 0$$

и значит, S_z -это нулевая компонента векторного оператора в стандартном представлении, и согласно теореме Вигнера-Эккарта

$$\langle J, M_J \,|S_m|\, J, M'_J\rangle = \frac{\langle J\|S\|J\rangle}{\sqrt{2J+1}}\langle J, M_J|J, M'_J; 1, m\rangle\,, \quad m = \{z, \pm\}$$

где коэффициент Клебша-Гордона отличен от нуля при $J \neq 0$ (правило запрета переходов $0 \to 0'$ за счет тензоров, не являющихся скалярами).

В этом параграфе мы будем иметь ввиду это условие.

Совершенно аналогично для полного момента

$$\langle J, M_J \left| J_m \right| J, M'_J \rangle = \frac{\langle J \| J \| J \rangle}{\sqrt{2J+1}} \langle J, M_J | J, M'_J; 1, m \rangle \,, \quad m = \{z, \pm\}$$

откуда заключаем, что для одного и того жсе терма оператор полного спина S пропорциОН а.Лен оператору полного момента $\boldsymbol{J}$:

$$\boldsymbol{S} = \lambda \boldsymbol{J}$$

где параметр λ определяется значениями приведенных матричных элементов для заданного терма

$$\lambda = \frac{\langle J \| S \| J \rangle}{\langle J \| J \| J \rangle}$$

и не зависит от вели чины проекции M_J. Определим λ, рассчитав матри чные элементы

$$\langle (\boldsymbol{S} \cdot \boldsymbol{J}) \rangle = \lambda \left\langle \boldsymbol{J}^2 \right\rangle \quad \to \quad \left\langle (\boldsymbol{L} \cdot \boldsymbol{S}) + \boldsymbol{S}^2 \right\rangle = \lambda J(J+1)$$

откуда

$$\lambda = \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}$$

В итоге, матричный элемент возмущения

$$\langle V_{\text{mag.}} \rangle = \mu_0 \mathcal{H} M_J g_{\text{LSJ}}$$

где фактор Ланде

$$g_{\text{LSJ}} = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}$$

В терминах ларморовской частоты $\Omega = e\mathcal{H}/(2mc)$ расщепление уровней В терме

$$\epsilon_1 \left(M_J \right) = \hbar \Omega g_{\text{LSJ}} M_J$$

Итак, атомный терм в слабом магнитном поле расщепляется на $2J+1$ уровней, т.е. вырождение терма сним ается полностью.

14.2.5 Zeeman effects: other topics

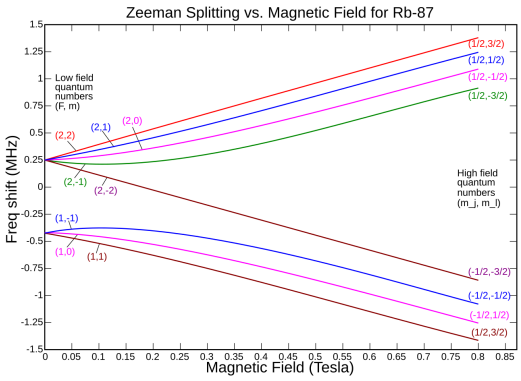
Intermediate Zeeman effect or why one level ran away?

(for now it is a question, later I'll think more about it!)

What happens in intermediate fields?

why one level ran away?

(see wiki for it)



(???)

14.2.6 Hyperfine interactions: basics

Основные формулы (??)

мотивация

где встречается?
что дает?

модель сверхтонкого расщепления

(задача из Белоусова по сути)
(мб уже это было раньше обсуждено????)
Гамильтониан

$$H = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{r} - (\boldsymbol{\mu} \cdot \mathbf{H}) \equiv H_0 + V, \quad V = -(\boldsymbol{\mu} \cdot \mathbf{H})$$

где

$$\mu = -\mu_0 \sigma_e, \quad \mathbf{H} = \operatorname{rot} A$$

Как известно из теории поля,

$$A = \frac{(\mu_p \times \mathbf{r})}{r^3} = -(\mu_p \times \nabla)\frac{1}{r}, \quad \mu_p = \mu_p \sigma_p$$

Подставляя (17.3) в (17.2), получаем

$$\mathbf{H} = -(\nabla \times (\mu_p \times \nabla))\frac{1}{r}$$

откуда

$$V = -\mu_0 \mu_p \sigma_e (\nabla \times (\sigma_p \times \nabla))\frac{1}{r}$$

Преобразуем немного $(\nabla \times (\sigma_p \times \nabla))_\alpha$:
$(\nabla \times (\sigma_p \times \nabla))_\alpha = \epsilon_{\alpha\beta\gamma}\nabla_\beta \epsilon_{\gamma\mu\nu}\sigma_p^\mu \nabla_\nu = (\delta_{\alpha\mu}\delta_{\beta\nu} - \delta_{\alpha\nu}\delta_{\beta\mu})\nabla_\beta \sigma_p^\mu \nabla_\nu = (\sigma_p \Delta - (\sigma_p \cdot \nabla)\nabla)_\alpha$

Тогда возмущение примет вид

$$V = -\mu_0 \mu_p \sigma_e (\sigma_p \Delta - (\sigma_p \cdot \nabla)\nabla)\frac{1}{r}$$

Поправка к энергии основного состояния атома водорода с возмущением (17.5) вычисляется по формуле

$$\epsilon_1 = \int d_3 x \psi^\dagger \left(\mathbf{r}, s_e, s_p\right) V \psi \left(\mathbf{r}, s_e, s_p\right)$$

Волновая функция нулевого приближения факторизуется в произведение пространственной и спиновой волновых функций

$$\psi \left(\mathbf{r}, s_e, s_p\right) = \psi_{100}(\mathbf{r}) \cdot \chi \left(s_e, s_p\right), \quad \psi_{100}(\mathbf{r}) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

Интегрирование выражения (17.6) по углам в сферических координатах даёт нам выражение, в котором необходимо $\nabla_\alpha \nabla_\beta$ заменить на $\frac{1}{3}\delta_{\alpha\beta}\triangle$, то есть

$$\epsilon_1 = -\frac{2}{3}\mu_0\mu_p \int dr |\psi_{100}(\mathbf{r})|^2 \chi^\dagger \sigma_e \cdot \sigma_p \chi \Delta \frac{1}{r}$$

Учитывая, что $\triangle \frac{1}{r} = -4\pi\delta(\mathbf{r})$, получаем

$$\epsilon_1 = \frac{8\pi}{3}\mu_0\mu_p \left|\psi_{100}(0)\right|^2 \chi^\dagger \sigma_e \cdot \sigma_p \chi = \frac{8\pi}{3}\mu_0\mu_p \frac{1}{\pi a^3} \chi^\dagger \sigma_e \cdot \sigma_p \chi$$

Проведём теперь усреднение по спиновым волным функциям.

Суммарный спин

$$s = s_e + s_p$$

то есть

$$s^2 = s_e^2 + s_p^2 + 2\left(s_e \cdot s_p\right) = \tfrac{1}{2}\left(\tfrac{1}{2}+1\right) + \tfrac{1}{2}\left(\tfrac{1}{2}+1\right) + \tfrac{1}{2}\left(\sigma_e \cdot \sigma_p\right) = \tfrac{3}{2} + \tfrac{1}{2}\left(\sigma_e \cdot \sigma_p\right)$$
$$\left(\sigma_e \cdot \sigma_p\right) = 2s^2 - 3$$

Подставляя (17.9) в (17.8), находим

$$\epsilon_1 = \epsilon_1(s) = \frac{8}{3a^3}\mu_0\mu_p[2s(s+1) - 3]$$

где $s = 0; 1$.

Значит,

$$\epsilon_1(0) = -\frac{8}{a^3}\mu_0\mu_p, \quad \epsilon_1(1) = \frac{8}{3a^3}\mu_0\mu_p$$

Таким образм, исходный уровень расщепляется на два в соответствии со значением суммарного спина (см. (17.10) и (17.11)), причём один из этих уровней трёхкратно вырожден ($s = 1, m = 0, \pm 1$), а другой - невырожденный ($s = 0$). Частота перехода

$$\nu = \frac{\epsilon_1(1) - \epsilon_1(0)}{h} = 1417 \text{ Hz}$$

14.2.7 Hyperfine interactions: other topics

О другом про сверхтонкую структуру (!?!??)

(там много всего есть, потом укажу многое.)

14.3 Fundamentals of Atomic Physics

(пока об этом в записи по атомной физике)

14.3.1 Influence of the Solid-State Lattice on the Atom (????)

(not the most important question, but it is very interesting, and I don't know answers yet about it)

(подробно обсужу, почему некоторые магнитные свойства от нее теряются и как вообще так, что у нас есть стабильные материалы? казалось бы, никакой структуры и не должно быть, никаких решеток. пока оставил этот вопрос.)

14.4 Other on Quantum Scattering Theory

(тут многие другие темы, нпр из ЛЛ3. супер редко они нужны, так что раздел и вдали.)

14.4.1 Gell-Mann and Low theorem

(пока по вики)

Statement of the theorem

Let $|\Psi_0\rangle$ be an eigenstate of H_0 with energy E_0 and let the 'interacting' Hamiltonian be $H = H_0 + gV$, where g is a coupling constant and V the interaction term. We define a Hamiltonian $H_\epsilon = H_0 + e^{-\epsilon|t|}gV$ which effectively interpolates between H and H_0 in the limit $\epsilon \to 0^+$and $|t| \to \infty$. Let $U_{\epsilon I}$ denote the evolution operator in the interaction picture. The Gell-Mann and Low theorem asserts that if the limit as $\epsilon \to 0^+$of

$$\left|\Psi_\epsilon^{(\pm)}\right\rangle = \frac{U_{\epsilon I}(0, \pm\infty)\,|\Psi_0\rangle}{\langle\Psi_0\,|U_{\epsilon I}(0, \pm\infty)|\,\Psi_0\rangle}$$

exists, then $\left|\Psi_\epsilon^{(\pm)}\right\rangle$are eigenstates of H Note that when applied to, say, the ground-state, the theorem does not guarantee that the evolved state will be a ground state. In other words, level crossing is not excluded.

Proof

As in the original paper, the theorem is typically proved making use of Dyson's expansion of the evolution operator. Its validity however extends beyond the scope of perturbation theory as has been demonstrated by Molinari. We follow Molinari's method here. Focus on H_ϵ and let $g = e^{\epsilon\theta}$. From Schrdinger's equation for the time-evolution operator

$$i\hbar\partial_{t_1} U_\epsilon(t_1, t_2) = H_\epsilon(t_1)\, U_\epsilon(t_1, t_2)$$

and the boundary condition $U_\epsilon(t_2, t_2) = 1$ we can formally write

$$U_\epsilon(t_1, t_2) = 1 + \frac{1}{i\hbar}\int_{t_2}^{t_1} dt' \left(H_0 + e^{\epsilon(\theta - |t'|)}V\right) U_\epsilon(t', t_2)$$

Focus for the moment on the case $0 \geq t_1 \geq t_2$. Through a change of variables $\tau = t' + \theta$ we can write

$$U_\epsilon(t_1, t_2) = 1 + \frac{1}{i\hbar}\int_{\theta+t_2}^{\theta+t_1} d\tau \left(H_0 + e^{\epsilon\tau}V\right) U_\epsilon(\tau - \theta, t_2)$$

We therefore have that

$$\partial_\theta U_\epsilon(t_1,t_2) = \epsilon g \partial_g U_\epsilon(t_1,t_2) = \partial_{t_1} U_\epsilon(t_1,t_2) + \partial_{t_2} U_\epsilon(t_1,t_2)$$

This result can be combined with the Schrdinger equation and its adjoint

$$-i\hbar\partial_{t_1} U_\epsilon(t_2,t_1) = U_\epsilon(t_2,t_1) H_\epsilon(t_1)$$

to obtain

$$i\hbar\epsilon g\partial_g U_\epsilon(t_1,t_2) = H_\epsilon(t_1) U_\epsilon(t_1,t_2) - U_\epsilon(t_1,t_2) H_\epsilon(t_2)$$

The corresponding equation between $H_{\epsilon I}, U_{\epsilon I}$ is the same. It can be obtained by pre-multiplying both sides with $e^{iH_0 t_1/\hbar}$, post-multiplying with $e^{iH_0 t_2/\hbar}$ and making use of

$$U_{\epsilon I}(t_1,t_2) = e^{iH_0 t_1/\hbar} U_\epsilon(t_1,t_2) e^{-iH_0 t_2/\hbar}$$

The other case we are interested in, namely $t_2 \geq t_1 \geq 0$ can be treated in an analogous fashion and yields an additional minus sign in front of the commutator (we are not concerned here with the case where $t_{1,2}$ have mixed signs). In summary, we obtain

$$(H_{\epsilon,t=0} - E_0 \pm i\hbar\epsilon g\partial_g) U_{\epsilon I}(0,\pm\infty)|\Psi_0\rangle = 0$$

We proceed for the negative-times case. Abbreviating the various operators for clarity

$$i\hbar\epsilon g\partial_g (U|\Psi_0\rangle) = (H_\epsilon - E_0) U|\Psi_0\rangle$$

Now using the definition of Ψ_ϵ we differentiate and eliminate derivatives $\partial_g(U|\Psi_0\rangle)$ using the above expression, finding

$$\begin{aligned} i\hbar\epsilon g\partial_g|\Psi_\epsilon\rangle &= \frac{1}{\langle\Psi_0|U|\Psi_0\rangle}(H_\epsilon - E_0) U|\Psi_0\rangle - \frac{U|\Psi_0\rangle}{\langle\Psi_0|U|\Psi_0\rangle}\langle\Psi_0|(H_\epsilon - E_0)U|\Psi_0\rangle \\ &= (H_\epsilon - E_0)|\Psi_\epsilon\rangle - |\Psi_\epsilon\rangle\langle\Psi_0|H_\epsilon - E_0|\Psi_\epsilon\rangle \\ &= [H_\epsilon - E]|\Psi_\epsilon\rangle . \end{aligned}$$

where $E = E_0 + \langle\Psi_0|H_\epsilon - H_0|\Psi_\epsilon\rangle$. We can now let $\epsilon \to 0^+$as by assumption the $g\partial_g|\Psi_\epsilon\rangle$ in left hand side is finite. We then clearly see that $|\Psi_\epsilon\rangle$ is an eigenstate of H and the proof is complete.

Примеры применений (???)

(я не знаю, где эта теорема применяется, потому что почти не понял ее. напишу, если узнаю.)

14.4.2 Ramsauer Effect

(по идее тут должна быть достаточная теория, пока так)

Общефизическая теория

Эффект Рамзауэра это явление аномально слабого рассеяния медленных электронов атомами нейтральных газов

К. Рамзауэр в 1921 году изучал рассеяние электронов в газообразном аргоне, и находил зависимость сечения упругого рассеяния электрона в зависимости от его энергии. Оказалось, что при уменьшении энергии меньших 16 эВ наблюдалось

уменьшение сечения практически до нуля с минимумом, достигаемым при энергии порядка 1 эВ, хотя в соответствии с классической механикой сечение должно возрастать.

Позднее аналогичные наблюдения были сделаны и для некоторых других тяжёлых газов.

Эффект также был косвенно подтверждён в опытах по измерению подвижности электронов в нейтральных газах.

(далее посмотрим на классическое и квантовое описание этого)

14.4.3 Other on Scattering Theory

14.5 Some Methods of Collisions and Scattering

(мб перенесу в часть выше, посмотрим)

14.5.1 Other on Elastic Collisions

(от Ландау тем много)

Амплитуда рассеяния в импульсном представлении

Рассеяние при больших энергиях

Рассеяние медленных частиц

Резонансное рассеяние при малых энергиях

Резонанс на квазидискретном уровне

Столкновения одинаковых частиц

Резонансное рассеяние заряженных частиц

Упругие столкновения быстрых электронов с атомами

Рассеяние при спин-орбитальном взаимодействии

Полюсы Редже

14.5.2 Other on Inelastic Collisions

(от Ландау тем много)

Упругое рассеяние при наличии неупругих процессов

Неупругое рассеяние медленных частиц

Матрица рассеяния при наличии реакций

Взаимодействие в конечном состоянии при реакциях

Неупругие столкновения быстрых электронов с атомами

Эффективное торможение

Неупругие столкновения тяжелых частиц с атомами

14.6 Fundamentals of Nuclear Physics

(see note on nuclear physics about it, there are many many books about it)

14.7 Electronic Magnetic Resonances

(???)

Основные формулы (??)

мотивация

отличие от других резонансов

в ядерной физике особенно подробно разные резонансы рассматриваются.

спиновое эхо (????)

интересное явление, изучу эпр, пото его просматривать буду
(а мб оно не связано с атомами? не знаю вот)

модель

связь с ЭПР

(??)

15 Open Quantum Systems, Many Particle Systems

Обсудим подробно открытые квантовые системы.

15.1 Typical Models of Open Quantum Systems (?)

15.1.1 Spin-Boson Model

Изучем на микроскопическом уровне динамику открытой системы, взаимодействующей с окружением. Изучать её мы будем на примере простейшей модели, которую можно придумать - так называемой спинбозонной модели (spin-boson model). Система (s, system) будет представлять собой двухуровневую систему (это может быть спин-1/2 в магнитном поле, это может быть частица в двухъямном потенциале - детали совершенно не важны), которую мы будем описывать на языке спина-1/2 и матриц Паули. В качестве модели окружающей среды (e, environment; также часто её называют баней - bath) мы возьмём набор гармонических осцилляторов. Гамильтониан всей системы имеет вид:

$$\hat{H} = \underbrace{-\frac{\Delta}{2}\hat{\sigma}_z}_{\hat{H}_s} + \underbrace{\sum_n \omega_n \hat{a}_n^\dagger \hat{a}_n}_{\hat{H}_e} + \underbrace{\hat{\sigma}_x \sum_n \lambda_n \hat{X}_n}_{\hat{V}}, \quad \hat{X}_n = \hat{a}_n + \hat{a}_n^\dagger$$

Такой вид взаимодействия обусловлен следующими простыми соображениями. Во-первых, ничего сложнее чем какаято линейная комбинация матриц Паули для двухуровневой системы предложить нельзя; поэтому взаимодействие линейно по $\hat{\boldsymbol{\sigma}}$; без ограничения общности [1] можно устроить взаимодействие именно посредством $\hat{\sigma}_z$. Во-вторых, мы будем предполагать, что отклонения осцилляторов от положения равновесия будут в каком-то смысле малы, и поэтому «сила» раскладывается линейно по отклонениям $\hat{X}$. Величины λ_n играют роль констант связи, которые будут предполагаться в каком-то смысле маленькими; по ним мы будем устраивать теорию возмущений.

В принципе, вся система s+e является замкнутой и допускает описание на языке волновых функций. Однако интересоваться мы будем именно динамикой двухуровневой системы, для описания которой необходимо ввести редуцированную матрицу плотности $\hat{\rho}_s(t) = \mathrm{Tr}_e\, \hat{\rho}(t)$, где $\hat{\rho}(t)$ - матрица плотности всей системы, а операция Tr_e подразумевает взятие частичного следа по степеням свободы окружающей среды. Полученный в результате такой операции объект - это матрица 2×2.

15.1.2 Interaction Representation of Open Systems

Работать мы будем в операторном формализме, используя представление взаимодействия по отношению к невозмущённому гамильтониану $\hat{H}_e + \hat{H}_s$ и с возмущением $\hat{V}$. Среда Динамика повышающих и понижающих операторов записывается просто:

$$\frac{d\hat{a}_n}{dt} = i\left[\hat{H}_e, \hat{a}_n\right] = i\left[\omega_n \hat{a}_n^\dagger \hat{a}_n, \hat{a}_n\right] = -i\omega_n \hat{a}_n \Rightarrow \hat{a}_n(t) = \hat{a}_n e^{-i\omega_n t}, \quad \hat{a}_n^\dagger(t) = \hat{a}_n^\dagger e^{i\omega_n t}$$

Система Для матриц Паули мы получаем:

$$\frac{d\hat{\sigma}_x}{dt} = i\left[\hat{H}_s, \hat{\sigma}_x\right] = \Delta\hat{\sigma}_y, \quad \frac{d\hat{\sigma}_y}{dt} = -\Delta\hat{\sigma}_x, \quad \frac{d\hat{\sigma}_z}{dt} = 0$$

и решение записывается как:

$$\begin{cases} \hat{\sigma}_x(t) = \hat{\sigma}_x \cos\Delta t + \hat{\sigma}_y \sin\Delta t \\ \hat{\sigma}_y(t) = -\hat{\sigma}_x \sin\Delta t + \hat{\sigma}_y \cos\Delta t \\ \hat{\sigma}_z(t) = \hat{\sigma}_z \end{cases}$$

Такая «тривиальная» невозмущённая эволюция тем самым описывает просто прецессию спина с угловой скоростью Δ вокруг направления «магнитного поля» z. Если же мы говорим, к примеру, о частице в двухъямном потенциале то такая когерентная прецессия соответствует осцилляциям Раби. В контексте спинов или кубитов, такое представление также часто называют приближением вращающейся волны (rotating wave approximation); это связано с тем, что в каком-то смысле оно эквивалентно переходу во вращающуюся систему отсчёта. Возмущение Соответственно, от гамильтониана с представлении взаимодействия остаётся только лишь возмущение. Последнее мы можем записать через один-единственный оператор «случайной силы» $\hat{\Phi}(t)$, с которой баня действует на нашу двухуровневую систему:

$$\hat{V}(t) = \hat{\sigma}_x(t)\hat{\Phi}(t), \quad \hat{\Phi}(t) = \sum_n \lambda_n \hat{X}_n(t)$$

В дальнейшем мы увидим, что явный вид «силы», который тут предложен, в действительности не сильно важен - а важны лишь определённые корреляционные функции этой силы.

15.1.3 Born–Markov Approximation

Полная матрица плотности в представлении взаимодействия удовлетворяет следующему уравнению:

$$\frac{d\hat{\rho}(t)}{dt} = i[\hat{\rho}(t), \hat{V}(t)]$$

Мы интересуемся следующей постановкой задачи. В начальный момент времени $t = 0$ баня находилась в равновесии с температурой T, и поэтому описывалась своей матрицей

плотности $\hat{\rho}_e(0) = \frac{1}{Z} e^{-\beta \hat{H}_e}$; а система была приготовлена со своей матрицей плотности $\hat{\rho}_s(0)$ (которая может соответствовать чистому состоянию $|\psi_0\rangle \langle\psi_0|$, или описывать смешанное состояние - сейчас это не очень важно); и изначально мы предполагаем, что баня и система никак не взаимодействовали, $\hat{\rho}(0) = \hat{\rho}_e(0) \otimes \hat{\rho}_s(0)$. В результате временной эволюции, происходит запутывание и матрица плотности больше не представляет собой простое тензорное произведение; поэтому, вообще говоря, не очень понятно, как брать частичный след в правой части уравнения (9.6).

Предлагается сделать несколько приближений. Первое приближение заключается в том, что если система достаточно маленькая, а среда - достаточно большая [2], то разумно считать, что матрица плотности среды практически не меняется с течением времени. Если мы, однако, предположим, что матрица плотности в произвольный момент времени выглядит как $\hat{\rho}(t) = \hat{\rho}_e \otimes \hat{\rho}_s(t)$, и возьмём в уравнении (9.6) частичный след, мы немедленно получим ноль в правой части; и связанно это с тем, что в равновесии средняя сила равна нулю:

$$\mathrm{Tr}_e \left(\hat{\rho}_e \hat{\Phi}(t) \right) \equiv \langle \hat{\Phi}(t) \rangle = \sum_n \lambda_n \left\langle \hat{X}_n(t) \right\rangle = 0$$

поэтому делать такое такое приближение наивно нельзя. Можно, однако, обойти эту трудность, сделав серию тождественных преобразований в уравнении (9.6): сперва мы его проинтегрируем от какого-то произвольного момента времени t_0 до t, а затем полученное выражение подставим опять в правую часть уравнения [3]:

$$\hat{\rho}(t) = \hat{\rho}\left(t_0\right) + i \int\limits_{t_0}^{t} dt' \left[\hat{\rho}\left(t'\right), \hat{V}\left(t'\right) \right] \Rightarrow \frac{d\hat{\rho}(t)}{dt} = i \left[\hat{\rho}\left(t_0\right), \hat{V}(t) \right] - \int\limits_{t_0}^{t} dt' \left[\left[\hat{\rho}\left(t'\right), \hat{V}\left(t'\right) \right], \hat{V}(t) \right]$$

В этом уравнении уже можно взять частичный след, предположив матрицу плотности в таком виде. Идеологически то что было сейчас проделано - это второй порядок теории возмущений по $\hat{V}$, и сделанное приближение носит название Борновского приближения. Беря частичный след слева и справа, и переходя к $\tau = t - t'$, мы получаем:

$$\frac{d\hat{\rho}_s}{dt} = - \int\limits_{0}^{t-t_0} d\tau \, \mathrm{Tr}_e \left(\left[\left[\hat{\rho}_s(t-\tau) \hat{\rho}_e, \hat{V}(t-\tau) \right], \hat{V}(t) \right] \right)$$

Как мы продемонстрируем далее явно, в результате взятия частичного следа возникнут корреляционные функции вида $S\left(t - t'\right) \equiv \left\langle \hat{\Phi}(t) \hat{\Phi}\left(t'\right) \right\rangle$ (несложно видеть, они зависят только от разности времён). Такие автокорреляционные функции определяются динамикой среды, и как правило, они быстро спадают до нуля на очень малых масштабах времени - если окружающая среда содержит огромное количество степеней свободы, то о корреляциях на сколь либо продолжительных временах говорить не приходится. Это приближение носит название Марковского приближения, и сводится оно к следующему физическому свойству окружающей среды - как правило, среда не обладает памятью.

Если предположить, что этот масштаб времени много меньше масштаба времени, на котором меняется сама матрица плотности, то можно заменить $\hat{\rho}_s(t-\tau) \mapsto \hat{\rho}_s(t)$, а также в силу сходимости интеграла, заменить его верхний предел до бесконечности. В результате мы получаем следующее квантовое кинетическое уравнение (master equation):

$$\frac{d\hat{\rho}_s}{dt} = - \int\limits_{0}^{\infty} d\tau \, \mathrm{Tr}_e \left(\left[\left[\hat{\rho}_s(t) \hat{\rho}_e, \hat{V}(t-\tau) \right], \hat{V}(t) \right] \right)$$

В таком виде это - система линейных дифференциальных уравнений с постоянными коэффициентами на компоненты матрицы плотности $\hat{\rho}_s$. Если окружающая среда не обладает памятью, то самый общий вид квантового кинетического уравнения имеет вид уравнения Линблад **a**[4]:

$$\frac{d\hat{\rho}_s(t)}{dt} = i\left[\hat{\rho}_s(t), \hat{H}_s\right] + \mathcal{L}\hat{\rho}_s(t)$$

В правой части стоит супероператор - линейный оператор, действующий на пространстве линейных операторов носящий название оператора Линблада; он имеет смысл аналога интеграла столкновений в обычном кинетическом уравнении. Оператор этот не может быть произвольным - даже при взаимодействии с окружающей средой, такое уравнение должно сохранять нормировку $\operatorname{Tr}\hat{\rho}_s(t) = 1$ и положительную определённость матрицы $\hat{\rho}_s$. То что мы сейчас получили - это явный вид оператора Линблада в приближении Борна-Маркова.

Явный вид

Чтобы продвинуться дальше, давайте подставим явный вид возмущения и раскроем коммутаторы:

$$\frac{d\hat{\rho}_s}{dt} = -\int_0^\infty d\tau \operatorname{Tr}_e\Big(\hat{\rho}_s(t)\underline{\hat{\rho}_e}\hat{\sigma}_x(t-\tau)\underline{\hat{\Phi}(t-\tau)}\hat{\sigma}_x(t)\underline{\hat{\Phi}(t)} - \hat{\sigma}_x(t-\tau)\underline{\hat{\Phi}(t-\tau)}\hat{\rho}_s(t)\underline{\hat{\rho}_e}\hat{\sigma}_x(t)\underline{\hat{\Phi}(t)}$$
$$-\hat{\sigma}_x(t)\underline{\hat{\Phi}(t)}\hat{\rho}_s(t)\underline{\hat{\rho}_e}\hat{\sigma}_x(t-\tau)\underline{\hat{\Phi}(t-\tau)} + \hat{\sigma}_x(t)\underline{\hat{\Phi}(t)}\hat{\sigma}_x(t-\tau)\underline{\hat{\Phi}(t-\tau)}\hat{\rho}_s(t)\underline{\hat{\rho}_e}\Big)$$

Подчёркнуты операторы, которые действуют на степени свободы окружающей среды (и которые, собственно, участвуют в операции взятии следа). При взятии следа мы: - можем как угодно менять местами подчёркнутые и не подчёркнутые операторы - ведь они действуют на разные степени свободы, и потому коммутируют. - не можем менять относительный порядок подчёркнутых операторов (аналогично и с не подчёркнутыми) - их коммутатор в общем случае отличен от нуля. - можем циклически переставлять подчёркнутые операторы как хотим - из-за операции взятии следа

Наконец, введя следующие корреляционные функции:

$$S_>(\tau) = \operatorname{Tr}_e\left(\hat{\rho}_e\hat{\Phi}(t)\hat{\Phi}(t-\tau)\right), \quad S_<(\tau) \equiv \operatorname{Tr}_e\left(\hat{\rho}_e\hat{\Phi}(t-\tau)\hat{\Phi}(t)\right) = S_>(-\tau)$$

мы можем избавиться от частичного следа и получить:

$$\frac{d\hat{\rho}_s}{dt} = -\int_0^\infty d\tau \left(S_<(\tau)\left[\hat{\rho}_s(t)\hat{\sigma}_x(t-\tau)\hat{\sigma}_x(t) - \hat{\sigma}_x(t)\hat{\rho}_s(t)\hat{\sigma}_x(t-\tau)\right] + S_>(\tau)\left[\hat{\sigma}_x(t)\hat{\sigma}_x(t-\tau)\hat{\rho}_s(t) - \hat{\sigma}_x(t-\tau)\hat{\rho}_s\right.\right.$$

15.1.4 Correlation Functions of the Environment

Дальше нам необходимо научиться вычислять корреляционные функции среды:

$$S_>(t) = \langle\hat{\Phi}(t)\hat{\Phi}(0)\rangle = \sum_{nm}\lambda_n\lambda_m\left\langle\hat{X}_n(t)\hat{X}_m(0)\right\rangle = \sum_n\lambda_n^2\left\langle\left(\hat{a}_n e^{-i\omega_n t} + \hat{a}_n^\dagger e^{i\omega_n t}\right)\left(\hat{a}_n + \hat{a}_n^\dagger\right)\right\rangle = \sum_n\lambda_n^2\left(\left\langle\hat{a}_n\hat{a}_n^\dagger\right\rangle\right.$$

Тут мы воспользовались тем, что осцилляторы независимы - поэтому остаются только члены $n = m$; и что средние значения $\langle\hat{a}_n\hat{a}_n\rangle = \left\langle\hat{a}_n^\dagger\hat{a}_n^\dagger\right\rangle = 0$, поскольку матрица плотности

диагональна в представлении чисел заполнения:

$$\hat{\rho}_e^{(n)} = \frac{1}{Z_n} e^{-\beta\omega_n \hat{a}_n^\dagger \hat{a}_n} \equiv \frac{1}{Z_n} \sum_{k=0}^{\infty} |k\rangle\langle k| \cdot e^{-\beta\omega_n k}$$

Отличные от нуля средние - следующие:

$$\left\langle \hat{a}_n^\dagger \hat{a}_n \right\rangle = \frac{\sum\limits_{k=0}^{\infty} \left\langle k \left| \hat{a}_n^\dagger \hat{a}_n \right| k \right\rangle e^{-\beta\omega_n k}}{\sum\limits_{k=0}^{\infty} e^{-\beta\omega_n k}} \equiv \frac{\sum\limits_{k=0}^{\infty} k e^{-\beta\omega_n k}}{\sum\limits_{k=0}^{\infty} e^{-\beta\omega_n k}} = n_B(\omega_n) \equiv \frac{1}{e^{\beta\omega_n} - 1}, \quad \left\langle \hat{a}_n \hat{a}_n^\dagger \right\rangle = \left\langle \hat{a}_n^\dagger \hat{a}_n \right\rangle + 1$$

Поскольку числа заполнения являются функциями энергии, то можно заметить, что вся информация о среде содержится в следующей функции - так называемой спектральной плотности среды:

$$J(\omega) \equiv \pi \sum_n \lambda_n^2 \delta(\omega - \omega_n)$$

Континуальный предел для среды как раз будет представлять собой замену $J(\omega)$ на некоторую непрерывную функцию частоты; её явный вид мы обсудим позже, а пока перепишем корреляционную функцию среды в следующем виде:

$$S_>(t) = \int_0^\infty \frac{d\omega}{\pi} J(\omega) \left((n_B(\omega) + 1) e^{-i\omega t} + n_B(\omega) e^{i\omega t} \right) \Rightarrow S_>(\omega) = 2\widetilde{J}(\omega) (n_B(\omega) + 1)$$

$$S_<(t) = \int_0^\infty \frac{d\omega}{\pi} J(\omega) \left(n_B(\omega) e^{-i\omega t} + (n_B(\omega) + 1) e^{i\omega t} \right) \Rightarrow S_<(\omega) = 2\widetilde{J}(\omega) n_B(\omega)$$

где обозначено $\widetilde{J}(\omega) \equiv J(\omega) - J(-\omega)$ и использовано $n_B(\omega) + 1 = -n_B(-\omega)$.

15.1.5 Bloch Equations

В принципе, дальше можно было бы подставить явный вид матриц Паули в представлении взаимодействия, и получить систему из 4 уравнений на 4 компоненты матрицы плотности. Однако, более наглядным является представление Блоха, которое параметризует матрицу плотности произвольной двухуровневой системы при помощи вектора $\boldsymbol{n}$ согласно:

$$\hat{\rho}_s(t) = \frac{1}{2}(\hat{\mathbb{I}} + \boldsymbol{n}(t) \cdot \hat{\boldsymbol{\sigma}}(t)) = \frac{1}{2} \begin{pmatrix} 1 + n_z & n_- e^{-i\Delta t} \\ n_+ e^{i\Delta t} & 1 - n_z \end{pmatrix}, \quad \boldsymbol{n}(t) \equiv \mathrm{Tr}\left(\hat{\rho}_s(t) \hat{\boldsymbol{\sigma}}(t)\right) = \langle \hat{\boldsymbol{\sigma}}(t) \rangle_s$$

(у вектора наглядный физический смысл - он представляет собой вектор поляризации спина). Напишем уравнения на компоненты вектора $\boldsymbol{n}$:

$$\frac{d\boldsymbol{n}(t)}{dt} = \mathrm{Tr}\left(\frac{d\hat{\boldsymbol{\sigma}}(t)}{dt} \hat{\rho}_s(t) \right) + \mathrm{Tr}\left(\hat{\boldsymbol{\sigma}}(t) \frac{d\hat{\rho}_s(t)}{dt} \right) = i \left\langle \left[\hat{H}_s, \hat{\boldsymbol{\sigma}}(t) \right] \right\rangle_s + \mathrm{Tr}\left(\hat{\boldsymbol{\sigma}}(t) \frac{d\hat{\rho}_s(t)}{dt} \right)$$

Первый член тривиален, он описывает когерентную прецессию в отсутствии взаимодействия, см. (9.3); поэтому мы сфокусируемся на втором члене, подставив в него (9.14), а также все операторы в представлении взаимодействия; исследуем что получилось покомпонентно. Сразу отметим, что уравнение на x-компоненту тривиально $-\frac{dn_x^{(2)}}{dt} = 0$. Связано это с тем, что $\left[\hat{\sigma}_x, \hat{V} \right] = 0$ - и поэтому точное уравнение имеет вид:

$$\frac{dn_x(t)}{dt} = -\Delta n_y(t)$$

Z-компонента

Подставляя и упрощая, получаем:

$$\frac{dn_z^{(2)}(t)}{dt} = -2\int\limits_0^\infty d\tau \left[n_z(t)S_K(\tau)\cos\Delta\tau - iS_R(\tau)\sin\Delta\tau\right]$$

где обозначены так называемые Келдышевские (K) и запаздывающие (R, retarded) корреляционные функции:

$$S_K(\tau) \equiv S_>(\tau)+S_<(\tau) \equiv \langle\{\hat\Phi(\tau),\hat\Phi(0)\}\rangle, \quad S_R(\tau) \equiv \theta(\tau)\left(S_>(\tau)-S_<(\tau)\right) \equiv \theta(\tau)\langle[\hat\Phi(\tau),\hat\Phi(0)]\rangle$$

Вычислим стоящие тут преобразования Фурье (используя тот факт, что $S_K(\tau)\equiv S_K(-\tau)$ и $2n_B(\omega)+1=\coth\frac{\beta\Delta}{2}$):

$$2\int\limits_0^\infty d\tau S_K(\tau)\cos\Delta\tau = S_K(\omega=\Delta) = 2J(\Delta)\coth\frac{\beta\Delta}{2}$$

$$2i\int\limits_0^\infty d\tau S_R(\tau)\sin\Delta\tau = S_>(\omega=\Delta)-S_<(\omega=\Delta) = 2J(\Delta)$$

Поэтому мы перепишем уравнение на z-компоненту в следующем виде:

$$\frac{dn_z(t)}{dt} = -\frac{n_z(t)-n_z^{(\mathrm{eq})}}{T_1}, \quad \frac{1}{T_1} = 2J(\Delta)\coth\frac{\beta\Delta}{2}, \quad n_z^{(\mathrm{eq})} = \tanh\frac{\beta\Delta}{2}$$

Это уравнение описывает процессы релаксации. Произвольное начальное значение намагниченности будет релаксировать за время T_1 (которое носит название времени релаксации) к своему равновесному значению $n_z^{(eq)}$ по закону $n_z(t) = n_z^{(eq)} + \left(n_z(0)-n_z^{(eq)}\right)e^{-t/T_1}$. Отметим, что величина $n_z^{(eq)}$ совпадает со средней «намагниченностью», если система, описываемая гамильтонианом $\hat H_s$, будет находится в термодинамическом равновесии с температурой, которая совпадает с температурой бани T. Тем самым, за время T_1 происходит термализация - устанавливается равновесие.

Для термализации необходимо, чтобы происходили реальные процессы переворота спина - при этом система должна забирать из бани (или отдавать туда) энергию Δ. Поэтому тот факт, что скорость релаксации оказалась пропорциональна $J(\Delta)$ - не удивительно; ведь если в окружающей среде, скажем, осцилляторы с частотой Δ отсутствовали бы, то было бы невозможно диссипировать в неё квант энергии Δ (во всяком случае, в первом порядке теории возмущений). Y-компонента Аналогично, путём прямых вычислений мы получаем:

$$\frac{dn_y^{(2)}(t)}{dt} = -2\int\limits_0^\infty d\tau S_K(\tau)\left(n_y(t)\cos\Delta\tau + n_x(t)\sin\Delta\tau\right)$$

Первый член уже был сосчитан ранее, а вот второй отличается - он не сводится к преобразованию Фурье и для его вычисления требуется регуляризация $e^{-\epsilon\tau}$ - которая, после использования формулы Сохоцкого, говорит нам, что оставшийся интеграл по частоте нужно брать в смысле главного значения:

$$2\int\limits_0^\infty d\tau S_K(\tau)\sin\Delta\tau = 2\int(d\omega)\widetilde J(\omega)\coth\frac{\beta\omega}{2}\int\limits_0^\infty d\tau e^{-i\omega\tau}\sin\Delta\tau = -\text{ v.p. }\int\limits_0^\infty\frac{d\omega}{\pi}J(\omega)\coth\frac{\beta\omega}{2}\frac{2\Delta}{\omega^2-\Delta^2}$$

Окончательно, собирая всё вместе, уравнение на y-компоненту выглядит следующим образом:

$$\frac{dn_y}{dt} = (\Delta - 2\delta)n_x(t) - \frac{n_y(t)}{T_2/2}, \quad \frac{1}{T_2} = J(\Delta)\coth\frac{\beta\Delta}{2}, \quad \delta = \text{ v.p.} \int\limits_0^\infty \frac{d\omega}{\pi} J(\omega)\coth\frac{\beta\omega}{2}\frac{2\Delta}{\omega^2-\Delta^2}$$

Выбор двоек в этом уравнении мотивирован следующим соображением. Полученная система линейных дифференциальных уравнений описывается следующей матрицей:

$$\frac{d}{dt}\begin{pmatrix} n_x \\ n_y \end{pmatrix} = \begin{pmatrix} 0 & -\Delta \\ \Delta - 2\delta & 2/T_2 \end{pmatrix}\begin{pmatrix} n_x \\ n_y \end{pmatrix}$$

которая имеет собственные частоты $\omega_{1,2} \approx \pm(\Delta - \delta) - \frac{i}{T_2}$. Поэтому величина δ - это поправка к частоте Δ, а затухание всех решений происходит как e^{-t/T_2}.

Вклад δ носит название Лэмбовского сдвига [5], он отвечает за перенормировку частоты «прецессии» Δ, связанную со взаимодействием с окружающей средой. В контексте двухъямного потенциала, Δ имеет смысл туннельного матричного элемента; тот факт, что δ уменьшает эффективную величину [6]Δ, является демонстрацией того, как взаимодействие с окружающей средой подавляет туннелирование. Хотя уравнения были написаны в рамках теории возмущений, можно показать, что в данной модели имеется квантовый фазовый переход - при достаточно сильном взаимодействии со средой, туннелирование подавляется до нуля.

Наконец, член T_2 носит название дефазировки, он подавляет поперечную компоненту $n_{x,y}(t)$ так, что они начинают затухать как e^{-t/T_2}. На этом характерном времени затухают когерентные осцилляции Раби. Имеется наглядный способ представить себе дефазировку. Давайте рассмотрим ансамбль спинов, вращающихся когерентно (синфазно) вокруг оси z с одинаковой частотой Δ. Однако, из-за взаимодействия с «шумом», индуцированным окружающей средой, частота каждого из этих спинов чуть «дрожит», из-за чего каждый из них начинает вращаться с чуть изменённой частотой. Хотя на малых временах эта поправка будет незаметна, и динамика будет оставаться когерентной - однако спустя какое-то время спины окажутся совершенно случайным образом разбросаны в плоскости, и среднее значение проекции спина на плоскость xy выйдет на нулевое значение.

Подчеркнём, что физически члены T_1 и T_2 имеют совершенно разную природу, и отвечают за различные физические процессы (хотя в рамках тривиальной теории возмущений и получилось, что они отличаются в два раза - в реальной жизни они могут быть совершенно различными; в частности, в домашней задаче будет предложена модель с отсутствующей релаксацией, но с наличием дефазировки). Грубо говоря, время T_2 - это время, в течение которого в нашей квантомеханической системе ещё могут наблюдаться какие-либо когерентные квантовые эффекты, и после которого система ведёт себя в большой мере классически. Время T_1 же говорит нам, когда измеряемые значения наблюдаемых перестанут зависеть от времени (разумеется, усреднив по быстрым квантовым осцилляциям).

15.1.6 On the Spectral Density

Всю информацию о структуре окружающей среды мы «спрятали» в спектральную функцию $J(\omega)$. С другой стороны, мы пока ничего не говорили о том, как $J(\omega)$ устроена. Она зависит от констант связи и от плотности состояний в бане; как правило, последняя растёт как какая-то степень частоты; как следствие, типичное поведение - это $J(\omega) \propto \omega^s$. С другой стороны, как правило в окружающей среде нельзя найти моды со сколь угодно большими частотами - у функции $J(\omega)$ может иметься обрезка на какой-то достаточно

большой частоте [7]ω_c, выше которой $J(\omega)$ быстро спадает до нуля. Наличие такой обрезки может быть существенно для некоторых эффектов, которые происходят от ультрафиолетовых степеней свободы бани (к примеру, при исследовании Лэмбовского сдвига). По поведению скорости релаксации при $\Delta \to 0$, выделяют несколько случаев:

- Омическая баня: $s = 1, J(\omega) = \pi\alpha\omega\theta(\omega_c - \omega)$. При этом $\frac{1}{T_{1,2}} \to \text{const}$ при $\Delta \to 0$. Наиболее часто встречаемый и простой тип «бани».
- Суб-омическая баня: $s < 1, \frac{1}{T_{1,2}} \to \infty$ при $\Delta \to 0$.
- Супер-омическая баня: $s > 1, \frac{1}{T_{1,2}} \to 0$ при $\Delta \to 0$.

15.2 Suppression of Tunneling in a Two-Level System

15.2.1 Perturbative Consideration

Исследуем чуть более подробно роль Лэмбовского сдвига δ, полученного для спин-бозонной модели ранее. Напомним, его роль заключается в подавлении матричного элемента $\Delta_{\text{eff}} = \Delta - \delta$, отвечающего туннельной амплитуде или частоте когерентных осцилляций Раби для двухъямного потенциала. Для простоты, мы будем исследовать случай нуля температур $T = 0$, и омическую баню $J(\omega) = \pi\alpha\omega\theta(\omega_c - \omega)$, считая $\omega_c \gg \Delta$. Прямое вычисление (9.30) даёт:

$$\delta = \text{ v.p.} \int_0^{\omega_c} \frac{d\omega}{\pi} \cdot \pi\alpha\omega \cdot \frac{2\Delta}{\omega^2 - \Delta^2} \approx 2\alpha\Delta \ln \frac{\omega_c}{\Delta}$$

Мы получили логарифмический интеграл, который набирается на всех масштабах, начиная от Δ и заканчивая ультрафиолетовой обрезкой на больших частотах ω_c (в отличие от всех предыдущих членов, которые определялись резонансным поведением - осцилляторами с частотами $\omega \approx \Delta$). Это значит, что несмотря на малость величины α, сам ответ δ вполне может оказаться сравним с Δ !

В старших порядках теории возмущений, вообще говоря, могут возникать такие же большие члены $\left(\alpha \ln \frac{\omega_c}{\Delta}\right)^n$; и если логарифм достаточно большой, то, по-хорошему, такие члены нужно учитывать все. Систематический способ учёта логарифмических расходимостей в рамках теории возмущений вплоть до бесконечных порядков возможен, и составляет суть метода ренормгруппы. С ним вы ознакомитесь позже, а здесь мы ограничимся более простым и физически наглядным способом, который приводит к такому же результату.

15.2.2 Adiabatic Consideration

Итак, мы получили логарифмическую поправку, которая приходит из широкого диапазона частот. Подавляющий вклад дают «быстрые» степени свободы бани с частотами $\omega_c \gg \omega \gg \Delta$.К счастью, когда имеется разделение быстрых и медленных степеней свободы, на помощь приходит адиабатическое приближение, которым можно воспользоваться и в этой задаче.

С точки зрения быстрых осцилляторов, удобно работать в базисе собственных состояний оператора $\hat{\sigma}_x$, соответствующих «частице в левой яме» $|\leftarrow\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \sigma_x = -1$ и «частице в правой яме» $|\rightarrow\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \sigma_x = +1($ в терминах двухъямного потенциала). Для анализа поведения системы, перепишем гамильтониан осцилляторов обратно в терминах операторов координаты $\hat{X} = \hat{a} + \hat{a}^\dagger$ и импульса $\hat{P} = \frac{\hat{a} - \hat{a}^\dagger}{2i}$, так что $[\hat{X}, \hat{P}] = i$: Итак, мы получили логарифмическую поправку,

которая приходит из широкого диапазона частот. Подавляющий вклад дают «быстрые» степени свободы бани с частотами $\omega_c \gg \omega \gg \Delta$. К счастью, когда имеется разделение быстрых и медленных степеней свободы, на помощь приходит адиабатическое приближение, которым можно воспользоваться и в этой задаче.

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$$\hat{a}_n^\dagger \hat{a}_n = \left(\frac{\hat{X}_n}{2} - i\hat{P}_n\right)\left(\frac{\hat{X}_n}{2} + i\hat{P}_n\right) = \hat{P}_n^2 + \frac{1}{4}\hat{X}_n^2 + \text{ const}$$

В таком случае, с точки зрения «быстрых» осцилляторов, нахождение частицы в левой или правой яме соответствует попросту сдвижке центра осциллятора:

$$\hat{H}_n \simeq \omega_n\left(\hat{P}_n^2 + \frac{1}{4}\hat{X}_n^2 \mp \frac{\lambda_n}{\omega_n}\hat{X}_n\right) = \omega_n\left(\hat{P}_n^2 + \frac{1}{4}\left[\hat{X}_n \mp 2\frac{\lambda_n}{\omega_n}\right]^2\right) + \text{ const}$$

и основное состояние такого «сдвинутого» осциллятора устроено как $e^{\pm i\hat{P}_n \cdot 2\frac{\lambda_n}{\omega_n}}|0_n\rangle$ (применили оператор трансляции). Поскольку быстрые осцилляторы «подстраиваются» под движение медленной двухуровневой подсистемы, с точки зрения «быстрых» осцилляторов полная волновая функция системы при этом соответствует следующей:

$$|\leftarrow\rangle_{\text{tot}} = |\leftarrow\rangle \otimes \prod_{\omega_n \gg \Delta} e^{2i\frac{\lambda_n}{\omega_n}\hat{P}_n}|0_n\rangle\,, \quad |\rightarrow\rangle_{\text{tot}} = |\rightarrow\rangle \otimes \prod_{\omega_n \gg \Delta} e^{-2i\frac{\lambda_n}{\omega_n}\hat{P}_n}|0_n\rangle\,,$$

где тензорное произведение берётся по всем осцилляторам бани. Из-за смещения осцилляторов из «бани», меняется также и эффективный матричный элемент, определяющий динамику двухуровневой системы: $\Delta_{\text{eff}} \equiv 2\left\langle \leftarrow \left| \hat{H}_{\text{spin}} \right| \rightarrow \right\rangle = \Delta \cdot \prod_{\omega_n \gg \Delta}\left\langle e^{-4i\frac{\lambda_n}{\omega_n}\hat{P}_n}\right\rangle_n$. Последнее произведение несложно вычислить (включая усреднение по основному состоянию осциллятора [8]), и получить:

$$\Delta_{\text{eff}} = \Delta \cdot \exp\left(-2\sum_{\omega_n \gg \Delta}\frac{\lambda_n^2}{\omega_n^2}\right) = \Delta \cdot \exp\left(-\frac{2}{\pi}\int\limits_{\omega \gg \Delta} d\omega \frac{J(\omega)}{\omega^2}\right) \simeq \Delta \cdot \exp\left(-2\alpha \ln\frac{\omega_c}{\Delta}\right)$$

В первом приближении это выражение совпадает с пертурбативным результатом (в пределе малых α), однако в этом выводе мы не накладывали никаких ограничений на α. Кроме того, заметим, что в действительности нижняя обрезка полученного логарифмического интеграла выбиралась из условия адиабатичности; поскольку реальная динамика двухуровневой подсистемы определяется именно Δ_{eff} , а не Δ, то это выражение нужно исправить и взять в качестве нижней обрезки именно $\Delta_{\text{eff.}}$ Это позволяет записать следующее уравнение самосогласования:

$$\Delta_{\text{eff}} = \Delta\left(\frac{\Delta_{\text{eff}}}{\omega_c}\right)^{2\alpha} \Rightarrow \Delta_{\text{eff}} = \Delta \cdot \left(\frac{\Delta}{\omega_c}\right)^{\frac{2\alpha}{1-2\alpha}}$$

Мы получили замечательный непертурбативный результат: в данной системе имеется квантовый фазовый переход при $\alpha = \frac{1}{2}$. При $\alpha < \frac{1}{2}$, система ведёт себя как квантовая

двухуровневая система, в ней наблюдается туннелирование и осцилляции Раби (с перенормированной частотой Δ_{eff}). Однако при достаточно сильной связи с окружающей средой, а именно, при $\alpha > \frac{1}{2}$, единственное решение уравнений самосогласования - это $\Delta_{\text{eff}} = 0$. Это означает полное подавление квантового туннелирования; с точки зрения двухъямного потенциала, частица, «посаженная» в одну из ям, там и остаётся.

15.2.3 Caldeira–Leggett Model

На этом семинаре мы обсудим микроскопическую модель диссипативной квантовой механики одной частицы, предложенную Калдейрой и Леггеттом. Заметим, что каким-нибудь тривиальным образом включить трение в квантовую механику не получится - гамильтонов формализм требует сохранения энергии и фазового объема. Но оказывается, что диссипативная механика получается естественным образом в системе частица-баня, как эффективная теория для частицы, полученная исключением степеней свободы бани [9]. При этом неизбежно возникает и второй компонент эффективного описания - случайная сила, действующая на частицу, характеристики которой, как мы увидим ниже, жёстко связаны с диссипативной частью. Гамильтониан мы запишем в следующем виде:

$$\hat{H} = \underbrace{\frac{\hat{P}^2}{2M} + V(\hat{X})}_{\hat{H}_s} + \underbrace{\sum_n \left(\frac{\hat{p}_n^2}{2m_n} + \frac{m_n \omega_n^2 \hat{x}_n^2}{2} \right)}_{\hat{H}_e} + \underbrace{\sum_n \left(-c_n \hat{x}_n \hat{X} + \frac{c_n^2}{2m\omega_n^2} \hat{X}^2 \right)}_{\hat{V}}$$

Величины c_n играют роль констант связи с баней. Член $\propto \hat{X}^2$ был написан для того, чтобы взаимодействие с осцилляторами «собиралось» в виде полного квадрата:

$$\frac{m_n \omega_n^2 \hat{x}_n^2}{2} - c_n \hat{x}_n \hat{X} + \frac{c_n^2}{2m\omega_n^2} \hat{X}^2 \equiv \frac{1}{2} m_n \omega_n^2 \left(\hat{x}_n - \frac{c_n}{m\omega_n^2} \hat{X} \right)^2$$

Такой гамильтониан «уважает» трансляционную инвариантность в случае отсутствия потенциала $V(X) = 0$ (сдвижка $X \mapsto X + a$, сопровождаемая сдвижкой $\hat{x}_n \mapsto \hat{x}_n + \frac{c_n}{m\omega_n^2} a$, оставляет гамильтониан инвариантным) - и поэтому, когда осцилляторы находятся в равновесии, средняя сила, действующая со стороны бани, равна нулю. Отклонение же любого из осцилляторов из положения равновесия вызывает дополнительную силу, действующую на исходную частицу.

Приближение Борна Маркова

Сперва обсудим, как можно было бы, по аналогии со спин-бозонной моделью, попробовать вывести кинетическое уравнение на матрицу плотности частицы, в приближении слабой связи. В предыдущей задаче мы могли выписать явно выписать невозмущённую динамику как системы, так и бани, что позволило нам обсудить поведение системы, когда характерные частоты бани и внутренней динамики системы одного порядка. Полностью аналогичное вычисление можно проделать для простых случаев, допускающих точное решение — к примеру, свободной частицы, осциллятора, линейного потенциала. Без указания явного вида потенциала, его проделать невозможно — мы попросту не сможем выписать представление взаимодействия для невозмущённой системы. Тем не менее,

Операторный формализм

мы можем это сделать в квазиклассическом пределе, когда динамика бани гораздо быстрее динамики системы - в таком случае достаточпо использовать прсдставлспис

взаимодсйствис только для бапи. УравIспии па матрицу плотпости в таком случае запишется в следующем виде:

$$\frac{d\hat{\rho}}{dt} = i\left[\hat{\rho}(t), \hat{H}_s\right] + i[\hat{\rho}(t), \hat{V}(t)], \quad \hat{V}(t) = \hat{\Phi}(t)\hat{X}, \quad \hat{\Phi}(t) = \sum_n c_n \hat{x}_n(t)$$

Дальнейший вывод производится так же - мы интегрируем это уравнение по отрезку $[t_0, t]$; дополнительное различие заключается в том, что мы подставляем полученное выражение для $\hat{\rho}(t)$ только во второе слагаемое. Наконец, беря след по степеням свободы бани, и используя тот факт, что корреляционные функции $\hat{\Phi}(t)$ локальны во времени, мы получаем кинетическое уравнение в несколько ином виде:

$$\frac{d\hat{\rho}_s}{dt} = i\left[\hat{\rho}_s(t), \hat{H}_s\right] - \int_0^\infty d\tau \,\mathrm{Tr}_e\left(\left[\left[\hat{\rho}_s(t)\hat{\rho}_e, \hat{V}(t-\tau)\right], \hat{V}(t)\right]\right)$$

Подчеркнём различие с предыдущим случаем - и сделанное дополнительное приближение. Тут имеется член, отвечающий динамике с $\hat{H}_s$, поскольку мы не производили переход в представление взаимодействия с $\hat{H}_s$; и в связи с этим, выражение для $\hat{V}(t)$ не содержит временную зависимость оператора координаты $\hat{X}$. Физически это отвечает квазиклассическому пределу - предположению о медленной динамике системы по сравнению с баней. Дальнейшее рассмотрение этого уравнение предлагается проделать в качестве домашнего упражнения.

Вместо этого мы будем исследовать операторные уравнения движения для частицы и осцилляторов - уравнения Гейзенберга. В действительности удобно писать уравнения на смещения $\hat{y}_n \equiv \hat{x}_n - \frac{c_n}{m\omega_n^2}\hat{X}$. Они имеют следующий вид:

$$\begin{cases} d\hat{X}/dt = \hat{P}/M \\ d\hat{P}/dt = -\partial V/\partial X + \sum_n c_n \hat{y}_n \end{cases}, \quad \begin{cases} d\hat{y}_n/dt = \hat{p}_n/m_n - \frac{c_n}{m\omega_n^2}\frac{d\hat{X}}{dt} \\ d\hat{p}_n/dt = -m_n\omega_n^2 \hat{y}_n \end{cases}$$

или, исключая импульсы:

$$M\frac{d^2\hat{X}}{dt^2} + \frac{\partial V}{\partial X} - \sum_n c_n \hat{y}_n = 0, \quad \frac{d^2\hat{y}_n}{dt^2} + \omega_n^2 \hat{y}_n = -\frac{c_n}{m\omega_n^2}\frac{d^2\hat{X}}{dt^2}$$

Наша задача - исключить степени свободы бани (осцилляторы) - и получить уравнения, описывающие движение только частицы. Это делается более или менее прямолинейно - уравнения движения среды линейны, и их можно решить с использованием классической функции Грина простого гармонического осциллятора $G_n(t) = \sin\omega_n t/\omega_n$, и используя интегрирование по частям:

$$\hat{y}_n(t) = \hat{y}_n(0)\dot{G}_n(t) + \left(\frac{\hat{p}_n(0)}{m_n} - \frac{c_n}{m\omega_n^2}\frac{d\hat{X}(0)}{dt}\right)G_n(t) - \frac{c_n}{m\omega_n^2}\int_0^t G_n(t-\tau)\frac{d^2\hat{X}(\tau)}{d\tau^2}d\tau$$

$$= \hat{y}_n(0)\dot{G}_n(t) + \frac{\hat{p}_n(0)}{m_n}G_n(t) - \frac{c_n}{m\omega_n^2}\int_0^t \dot{G}_n(t-\tau)\frac{d\hat{X}(\tau)}{d\tau}d\tau$$

Подставляя и группируя члены, мы можем записать уравнение на координату частицы в следующем виде:

$$M\frac{d^2\hat{X}}{dt^2} + \int_0^t \gamma(t-\tau)\frac{d\hat{X}(\tau)}{d\tau}d\tau + \frac{\partial V}{\partial X} = \hat{\zeta}(t), \quad \gamma(t) = \sum_n \frac{c_n^2}{m\omega_n^2}\dot{G}_n(t), \quad \hat{\zeta}(t) = \sum_n c_n\left(\hat{y}_n(0)\dot{G}_n(t) + \frac{\hat{p}_n(0)}{m_n}G_n\right.$$

Величина $\hat{\zeta}(t)$ выглядит как эффективная дополнительная сила, действующая на частицу и определяемая степенями свободы бани - в классической механике такого рода силы называют Ланжевеновскими. Член, зависящий от первой производной, несёт чисто диссипативный характер - он устроен как вязкое трение и приводит к несохранению энергии. Его нелокальность во времени отвечает «памяти» среды.

15.2.4 Spectral Weight and Ohmic Bath (???)

Как и ранее, всю информацию о степенях свободы бани, и о константах связи бани с частицей, можно «закодировать» в спектральной функции:

$$J(\omega) = \pi \sum_n \frac{c_n^2}{2m\omega_n} \delta(\omega - \omega_n) \Rightarrow \gamma(t) = \frac{2}{\pi} \int_0^\infty \frac{d\omega}{\omega} J(\omega) \cos \omega t$$

Другой важной характеристикой является корреляционная функция ланжевеновских сил [10], вычислить которую мы можем используя равновесные значения для осцилляторов

$$\left\langle \hat{y}_n^2 \right\rangle = \frac{1}{2m_n\omega_n} \coth \frac{\beta\omega_n}{2}, \quad \left\langle \hat{p}_n^2 \right\rangle = \frac{m_n\omega_n}{2} \coth \frac{\beta\omega_n}{2},$$

$$\left\langle \hat{\zeta}(t)\hat{\zeta}(t') \right\rangle = \sum_n \frac{c_n^2}{m\omega_n} \frac{1}{2} \coth \frac{\beta\omega}{2} \cos \omega (t - t') = \frac{1}{\pi} \int_0^\infty d\omega J(\omega) \coth \frac{\beta\omega}{2} \cos \omega (t - t')$$

Рассмотрим теперь случай омической бани $J(\omega) = \eta\omega$. Тогда:

$$\gamma(t) = \frac{2\eta}{\pi} \int_0^\infty d\omega \cos \omega t = 2\eta\delta(t)$$

Стоит быть аккуратным, поскольку в интеральном члене дельта-функция попадает ровно на границу области интегрирования, поэтому интеграл требует дополнительной регуляризации. В данном случае мы понимаем, что при внесении любой ультрафиолетовой обрезки для $J(\omega)$, функция $\gamma(t)$ останется чётной функцией времени. Поскольку она будет также являться узким пиком как функции времени, ровно половина этого пика войдёт в интеграл; это соответствует регуляризации типа $\int_0^t \delta(t-\tau)d\tau = \frac{1}{2}$:

$$M\frac{d^2\hat{X}}{dt^2} + \eta\frac{d\hat{X}}{dt} + \frac{\partial V}{\partial X} = \hat{\zeta}(t)$$

Кроме того, в высокотемпературном пределе $\coth \frac{\beta\omega}{2} \approx \frac{2T}{\omega}$, и это выражение прямо пропорционально «диссипативному ядру» и температуре: $\left\langle \hat{\zeta}(t)\hat{\zeta}(t') \right\rangle \approx T\gamma(t - t')$. В общем случае несложно видеть, что их Фурье-гармоники связаны друг с другом, что выражает собой флуктуационно-диссипационную теорему (ФДТ).

Данное уравнение является главным результатом семинара. Мы рассмотрели микроскопическую модель квантовомеханической диссипативной системы, и получили операторное уравнение, описывающее динамику частицы. От «бани» пришли две важных части - диссипация, или трение, и флуктуирующая возмущающая коротко коррелированная сила $\hat{\zeta}(t)$, коррелятор которой специальным образом связан с трением.

О случаях применения (!??!?)

(оставшийся вопрос)

Именно эти модели дают подготовку к кинетике

(проверю, чтобы там именно этот раздел и использовался. пока что связка слабая, потому что не писал этот раздел.)

15.3 Many Particle Systems [see cond matter]

[see cond matter for now about it. It is very much not a QM, but later I'll add intro.]

16 Quantum Optics, Quantum Information

(потом напишу, пока см. отдельную запись по квантовой оптике)

16.1 Quantum Entanglement

начинать нужно с википедии

Мысленный эксперимент Greenberger-Horne-Zeilinger-Mermin

говорят, понадобится это в понимании матрицы плотности, но я хз, потом подумаю.
мда.

объяснения Брайна Грина и теории струн

квантовая нелокальность, которая происходит при распутывании квантовых состояний совершенно непонятна и поэтому есть много их объяснений.

Брайн Грин утверждает, что пространства и время не являются фундаментальными элементами физического мира, а лишь следствиями первоначального отсутствия пространства.

Он сравнивает пространство с ковром, у которого есть потертости.
ткань мироздания..
и так из беспространства можно поизучать пространство.
Тим Модлин также писал много чего-то про это. философия физики у него там.
а может быть просто как говорил Эйнштейн, это просто не постижимо.

применение квантовой запутанности в квантовых компьютерах

как-то..

16.2 Fundamentals of Quantum Information Theory

(чуть потренирую и буду прописывать!!)

16.2.1 Introduction to Quantum Information Theory

(то, что Филиппов рассказывал, суть этого)

Основные понятия квантовой теории информации

программирование квантовых вычислений

16.2.2 Introduction to Quantum Computing (!!)

основа квантовых компьютеров, мб потом в главе про приложения это будет раскрыто лучше.

(тут очень крутые темы, до которых пока что я не дотягиваюсь. мб самая полезная из дополнительных тем квантовой механики.)

основы квантовых вычислений

мб запишу что-то с популярных лекций.

16.2.3 Introduction to Quantum Computers

Обсудим базовые вещи квантовых компьютеров.
(тут как раз эта ходовая теория)

Обзор квантовых компьютеров

польза квантовых компьютеров

Очень популярно рассказывать, как они работают и где они используются?
(пропишу от популярных видео, пока лень)
Важно разобраться, для чего они нужны, а для чего нет. А то тоже заблуждения есть про это.

пример алгоритма, который квантовый компьютер решает быстрее

я хз, интересно.

Главная идея квантовых компьютеров

я хз, как они работают

как догадаться до квантовых компьютеров?

Что там нужно знать из квантмеха, чтобы эта идея стала очевидна?
а я хз.

связь со сверхпроводниками

Говорят, квантовые компьютеры используют сверхпроводимость.
почему?

Кубиты и объекты из них

Кубиты - ключевая концепция квантовых компьютеров, так что продумаем их.

определение кубита

Мы должны уметь:
Инициализировать кубит
Поворачивать, то есть изменять состояние
Измерять

физическая реализация

хз, чем они реализованы?
Может быть реализована на основе спина

квантовый регистр

Введение в квантовые схемы

(тут из Лекций Филиппова суть и эта теория)

Типичные квантовые вентили и схемы

(коротко, раскрывая основную суть и приложения их укажу)

Вентиль Адамара

Вентиль Тоффли

Вентиль Фредкина

Квантовые вычисления

Что есть квантовое вычисление

И я хз на самом деле,
говорят, это как раз квантовая эволюция.
я хз.

16.3 Physical Realization of Ideas of Quantum Information

16.3.1 How to initialize and read the state of a qubit?

(????)

Part V
Problems in Quantum Mechanics

17 Problems of typical parts of quantum mechanics

17.1 Mastering typical methods

17.1.1 Problems about Time-Independent PT 1

ПТФ-7.з1. Поляризуемость частицы на кольце

Частица с массой M и зарядом e движется на кольце радиуса R. К системе прикладывается слабое электрическое поле $\mathcal{E}$ параллельно плоскости кольца. Определите поляризуемости $\alpha_n = -\frac{\partial^2 E_n}{\partial \mathcal{E}^2}$ всех уровней энергии.
Проведите вычисления, используя два различных базиса:
- Базис состояний с фиксированным угловым моментом m («волны де-Бройля»)
- Базис состояний с фиксированной чётностью

Указание: обратите внимание, что поскольку в задаче с приложенным электрическим полем чётность по-прежнему сохраняется, то для вычисления второго пункта применять вырожденную теорию возмущений нет необходимости.

Solution. в базисе состояний с фиксированным угловым моментом

$$\hat{p}^2 = -\hbar^2\Delta = -\frac{\hbar^2}{r^2}\frac{\partial^2}{\partial\varphi^2}$$

$$\hat{H}_0\psi = E_m^{(0)}\psi$$

$$-\frac{\hbar^2}{2M}\Delta\psi = E_m^{(0)}\psi \qquad \Rightarrow \qquad \psi_m(\varphi) = \frac{e^{im\varphi}}{\sqrt{2\pi}}; \qquad m \in \mathbb{Z}.$$

$\int_0^{2\pi} \psi_m^*\psi_{m'}d\varphi = \delta(m-m')$

$$E_m^{(0)} = \frac{m^2}{2MR^2}$$

Как видно, кратность вырождения энергии равна 2 (состояниям m и $-m$ соответствует энергия E_m).

$$\hat{H} = \hat{H}_0 + \hat{V} = -\frac{\hbar^2}{2MR^2}\frac{\partial^2}{\partial\varphi^2} - e\mathcal{E}R\cos\varphi$$

$$V_{\alpha\beta} \equiv \langle n_\alpha^{(0)}|\hat{V}|n_\beta^{(0)}\rangle = -e\mathcal{E}R\int_0^{2\pi}\cos\varphi e^{i(\beta-\alpha)\varphi}d\varphi = -\frac{1}{2}e\mathcal{E}R(\delta_{\beta-\alpha,1}+\delta_{\beta-\alpha,-1})$$

(since only $\int\cos^2(x) \neq 0$). $V_{\alpha\alpha} = 0$, и вырождение не снято, поэтому нужно рассматривать 2 порядок.
$\hat{H}^{(\text{eff})}_{\alpha\beta} = \sum\limits_{m\neq n}\frac{V_{\alpha m}V_{m\beta}}{\omega_{mn}}$, $\omega_{mn} = E_m^{(0)} - E_n^{(0)} = \frac{m^2-n^2}{2MR^2}$.

$$\hat{H}^{(\text{eff},n)}_{\alpha\beta} = e^2\mathcal{E}^2MR^4\begin{pmatrix} \frac{1}{4n^2-1} & \frac{\delta_{n,1}}{2} \\ \frac{\delta_{n,1}}{2} & \frac{1}{4n^2-1}\end{pmatrix}$$

$\det(\hat{H}^{(\text{eff})}_{\alpha\beta} - E_n^{(2)}) = 0 \qquad \Rightarrow$

$$E_1^{(2)} = -\frac{e^2\mathcal{E}^2MR^4}{6}, \qquad E_1^{(2)} = \frac{5e^2\mathcal{E}^2MR^4}{6}, \qquad E_n^{(2)} = \frac{e^2\mathcal{E}^2MR^4}{4n^2-1}$$

$$\alpha_{1(1)} = +\frac{e^2MR^4}{3}, \qquad \alpha_{1(2)} = -\frac{5e^2MR^4}{3}, \qquad \alpha_n = -\frac{2e^2MR^4}{4n^2-1}.$$

For $n = 0$ there is no degeneracy, so

$$V_{00} = 0$$
$$E_0^{(2)} = \sum_{m\neq 0} \frac{|V_{0n}|^2}{\omega_{0m}}$$
$$E_0^{(2)} = -e^2\mathcal{E}^2 MR^4$$
$$\alpha_0 = 2e^2 MR^4$$

Solution. в базисе состояний с фиксированной чётностью.

$$\psi_m^{(+)} = \frac{1}{\sqrt{\pi}}\cos(m\varphi), \qquad \psi_m^{(-)} = \frac{1}{\sqrt{\pi}}\sin(m\varphi)$$

$$V_{\alpha+,\beta+} = \frac{e\mathcal{E}R}{\varphi}\int_0^{2\pi}\cos(\varphi\alpha)\cos(\varphi\beta)\cos\varphi d\varphi = \frac{e\mathcal{E}R}{2}\left(\delta_{\alpha-\beta,1} + \delta_{\beta-\alpha,1} + \delta_{n+m,1}\right)$$

$$V_{\alpha-,\beta-} = \frac{e\mathcal{E}R}{\pi}\int_0^{2\pi}\sin(\varphi\alpha)\sin(\varphi\cdot\beta)\cos\varphi d\phi = \frac{e\mathcal{E}R}{2}\left(\delta_{\alpha-\beta,1} + \delta_{\alpha-\beta,1} - \delta_{\alpha+\beta,1}\right)$$

$$V_{\alpha-,\beta+} = \frac{e\mathcal{E}R}{\pi}\int_0^{2\pi}\sin(\varphi\alpha)\cos(\varphi\beta)\cos\varphi d\phi = 0 = V_{\alpha+,\beta-}$$

$$\hat{H}^{(\text{eff})}_{\alpha\beta} = \frac{e^2\mathcal{E}^2 MR^4}{\hbar^2}\begin{pmatrix} \frac{\delta_{n,1}}{2} + \frac{1}{4n^2-1} & 0 \\ 0 & -\frac{\delta_{n,1}}{2} + \frac{1}{4n^2-1}\end{pmatrix}$$

$\det(\hat{H}^{(\text{eff})}_{\alpha\beta} - E_n^{(2)}) = 0 \qquad \Rightarrow \qquad$ same answer.

В случае $n = 0$:

$$V_{0\beta,+} = \frac{e\mathcal{E}R}{\sqrt{2}}\delta_{n,1}, V_{0\beta,-} \equiv 0$$

Поправка к энергии получается такой же.

ПТФ-7.з2. Двуслойный графен

В силу решёточной структуры графена, волновая функция электронов представляет собой двухкомпонентный псевдоспинор $\psi(x) = (\psi_A(x), \psi_B(x))^T$, где различные компоненты отвечают различным подрешёткам. Возбуждения вблизи так называемой K-долины зоны Бриллюэна описываются эффективным гамильтонианом размера 2×2, который записывается следующим образом:

$$\hat{H} = v_F\hat{\vec{\sigma}}\cdot\hat{\vec{p}} = v_F(\hat{\sigma}_x\hat{p}_x + \hat{\sigma}_y\hat{p}_y) = v_F\begin{pmatrix} 0 & \hat{p}_x - i\hat{p}_y \\ \hat{p}_x + i\hat{p}_y & 0\end{pmatrix}$$

Для двуслойного графена, соответственно, волновая функция уже образует четырёхкомпонентный спинор

$$\psi(x) = (\psi_A^{(1)}(x), \psi_B^{(1)}(x), \psi_A^{(2)}(x), \psi_B^{(2)}(x))$$

Если бы между не было никакого взаимодействия, то гамильтониан системы имеет просто блочно-диагональный вид $\hat{H} = v_F\begin{pmatrix}\hat{\vec{\sigma}}\cdot\hat{\vec{p}} & 0 \\ 0 & \hat{\vec{\sigma}}\cdot\hat{\vec{p}}\end{pmatrix}$; однако, если два листа графена положить друг на друга определённым образом, то возникает возможность туннелирования электронов между слоями. Гамильтониан такой системы имеет вид:

$$\hat{H} = \begin{pmatrix} 0 & v_F(\hat{p}_x - i\hat{p}_y) & 0 & 0 \\ v_F(\hat{p}_x + i\hat{p}_y) & 0 & \Delta & 0 \\ 0 & \Delta & 0 & v_F(\hat{p}_x - i\hat{p}_y) \\ 0 & 0 & v_F(\hat{p}_x + i\hat{p}_y) & 0\end{pmatrix}$$

При нулевом импульсе p, матрица имеет двукратно вырожденное собственное число 0 и однократно вырожденные числа $\pm\Delta$. Если мы исследуем свойства возбуждений при маленькой энергии $|E| \ll \Delta$ и, соответственно, малом импульсе $p \ll \frac{\Delta}{v_F}$, то высокоэнергетические состояния $\pm\Delta$ несущественны.

Используя теорию возмущений, выведите эффективный гамильтониан, описывающий низкоэнергетические возбуждения, и определите спектр соответствующих двух зон.

Solution.

Пусть $a = v_F(\hat{p}_x - i\hat{p}_y)$.

$$w_{11} = w_{14} = 0, \quad w_{12} = \Delta, \quad w_{13} = -\Delta$$

1 порядок не убирает вырождение по энергии.
(???)

$$\hat{V} = v_F \begin{pmatrix} \hat{\vec{\sigma}} \cdot \hat{\vec{p}} & 0 \\ 0 & \hat{\vec{\sigma}} \cdot \hat{\vec{p}} \end{pmatrix}$$

$$H_{11}^{(1)} = \frac{V_{12}V_{21}}{\omega_{12}} + \frac{V_{13}V_{31}}{\omega_{13}} = -\frac{aa^\dagger}{\Delta}, \quad H_{14}^{(1)} = \frac{V_{12}V_{24}}{\omega_{12}} + \frac{V_{13}V_{34}}{\omega_{13}} = 0$$

$$H_{41}^{(1)} = \frac{V_{42}V_{21}}{\omega_{12}} + \frac{V_{13}V_{31}}{\omega_{13}} = 0, \quad H_{44}^{(1)} = \frac{V_{42}V_{24}}{\omega_{12}} + \frac{V_{43}V_{34}}{\omega_{13}} = \frac{aa^\dagger}{\Delta}$$

$$\hat{H}^{\text{eff}} = \frac{v_F^2 p^2}{\Delta} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\det(\hat{H}^{\text{eff}} - E_0^{(2)}) = 0 \to E_0^{(2)} = \pm \frac{p^2}{\Delta} v_F^2$$

Feigelman.EntrExam.th-2/8 2D particle in magnetic field

Charged particle those free Hamiltonian is $H = v\,(\sigma_x p_x + \sigma_y p_y)$ (where $\sigma_{x,y}$ are Pauli matrices) is moving in a magnetic field $\mathbf{B} = (0, 0, B)$. Find all eigenvalues and their degeneracies.

Solution

(???)

ПТФ-7.з3. Поляризуемость атома водорода

Атом водорода находится в основном состоянии, $\psi_{100}(r) = \frac{e^{-r/a}}{\sqrt{\pi a^3}}$, $a := \frac{\hbar^2}{me^2}$. Он помещается в постоянное электрическое поле, описываемое гамильтонианом $\hat{V} = -e\mathcal{E}\hat{z}$; требуется определить сдвиг уровня энергии и поляризуемость основного состояния.

Для расчёта сдвига энергии во втором порядке теории возмущений, вообще говоря, необходимо вычислять все матричные элементы $\langle 1,0,0|\hat{z}|n,l,m\rangle$, а кроме них ещё и матричные элементы $\langle 1,0,0|\hat{z}|k,l,m\rangle$ (k определяет энергию $\frac{\hbar^2 k^2}{2m} = E$) для состояний непрерывного спектра, а затем вычислять соответствующую сумму и интеграл. Это сложная задача; но, к счастью, тут можно поступить иначе. Для этого первую поправку по теории возмущений к волновой функции предлагается найти *точно*, а не искать её в виде разложения.

• Напишите точное уравнение для поправки первого порядка $\psi^{(1)}(r)$ по теории возмущений. Покажите, что в нём можно разделить переменные, сделав анзац $\psi^{(1)}(r,\theta) = f(r)e^{-r/a}\cos\theta$; напишите уравнение на функцию $f(r)$.
Hint: обезразмерьте это уравнение!

• Покажите, что это уравнение имеет простое полиномиальное решение $f(r) = A + Br + Cr^2$; найдите A, B, C.

• Найдя волновую функцию, вычислите поправку $E_{100}^{(2)}$ и поляризуемость α.

Замечание: альтернативный способ решения задачи об атоме водорода в постоянном электрическом поле — это использование параболических координат. Эти координаты замечательны в частности тем, что в них разделяются переменные и в электрическом поле; а кроме этого, лишь небольшое количество матричных элементов оператора $\hat{z}$ отлично от нуля. Именно благодаря этому обстоятельству поправка первого порядка и имеет такой простой вид.

Solution.

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{r}; \qquad \psi^{(0)}(r) = \frac{e^{-r/a}}{\sqrt{\pi a^3}}, \quad E^{(0)} = -\frac{e^2}{2a}; \qquad \hat{V} = -e\mathcal{E}\hat{z}$$

$$\psi = \psi^{(0)}(r) + \psi^{(1)}(r,\theta)$$

$$(\hat{H}_0 + \hat{V})(\psi^{(0)}(r) + \psi^{(1)}(r,\theta)) = (E^{(0)} + E^{(1)})(\psi^{(0)}(r) + \psi^{(1)}(r,\theta))$$

$$z = r\cos\theta$$

$$\hat{H}_0\psi^{(1)} + \hat{V}\psi^{(0)} = E^{(0)}\psi^{(1)}$$

$$-\frac{ae^2}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{1}{r^2}\operatorname{ctg}\theta\frac{\partial}{\partial\theta}\right)\psi^{(1)}(r,\theta) - \frac{e^2}{r}\psi^{(1)}(r,\theta) - \frac{e\mathcal{E}e^{-\frac{r}{a}}}{\sqrt{\pi a^3}}r\cos\theta = -\frac{e^2}{2a}\psi^{(1)}(r,\theta)$$

$$\psi^{(1)}(r,\theta) = f(r)e^{-r/a}\cos\theta$$

$$\frac{af''(r)}{2} + \frac{(a-r)f'(r)}{r} + \frac{r^2 - 2ar - 2a^2}{2ar^2}f(r) + \frac{f(r)}{r} + \frac{\mathcal{E}r}{e\sqrt{\pi a^3}} = \frac{f(r)}{2a}$$

$$\frac{af''(r)}{2} + \frac{(a-r)f'(r)}{r} - \frac{af(r)}{r^2} + \frac{\mathcal{E}r}{e\sqrt{\pi a^3}} = 0$$

$x := \frac{r}{a}$,

$$f''(x) + \frac{2(1-x)f'(x)}{x} - \frac{2f(x)}{x^2} + 2\sqrt{\frac{a}{\pi}}\frac{\mathcal{E}x}{e} = 0$$

$$f(x) \equiv A + Bx + Cx^2$$

$$C + \frac{(1-x)(B+2Cx)}{x} - \frac{A + Bx + Cx^2}{x^2} + \sqrt{\frac{a}{\pi}}\frac{\mathcal{E}x}{e} = 0$$

$$2C - B - 2Cx - \frac{A}{x^2} + \sqrt{\frac{a}{\pi}}\frac{\mathcal{E}x}{e} = 0$$

$$\begin{cases} A = 0, \\ 2C - B = 0. \\ C = \sqrt{\frac{a}{\pi}}\frac{\mathcal{E}}{2e} \end{cases}$$

$$A = 0, \quad B = \sqrt{\frac{a}{\pi}}\frac{\mathcal{E}}{e}, \quad C = \sqrt{\frac{a}{\pi}}\frac{\mathcal{E}}{2e}$$

$$f(x) = A + Bx + Cx^2 = \sqrt{\frac{a}{\pi}}\frac{\mathcal{E}x}{e}\left(1 + \frac{x}{2}\right)$$

$$\psi^{(1)}(r,\theta) = f(r)e^{-r/a}\cos\theta = \frac{\mathcal{E}r}{e\sqrt{\pi a}}\left(1 + \frac{r}{2a}\right)e^{-r/a}\cos\theta$$

2 порядок теории возмущений:

$$(\hat{H}_0 + \hat{V})(\psi^{(0)}(r) + \psi^{(1)}(r,\theta) + \psi^{(2)}(r,\theta)) = (E^{(0)} + E^{(2)})(\psi^{(0)}(r) + \psi^{(1)}(r,\theta) + \psi^{(2)}(r,\theta))$$

$$\hat{H}_0\psi^{(2)}(r,\theta) + \hat{V}\psi^{(1)}(r,\theta) = E^{(0)}\psi^{(2)}(r) + E^{(2)}\psi^{(0)}(r)$$

$$E^{(2)} = \langle\psi^{(0)}(r)|\hat{V}|\psi^{(1)}(r,\theta)\rangle = \int\limits_{-\pi}^{\pi} d\varphi \int\limits_{1}^{-1} d\cos\theta \int\limits_{0}^{\infty} dr r^2 \frac{e^{-r/a}}{\sqrt{\pi a^3}}(-e\mathcal{E}r\cos\theta)\frac{\mathcal{E}r}{e\sqrt{\pi a}}\left(1 + \frac{r}{2a}\right)e^{-r/a}\cos\theta = -\frac{9}{4}a^3\mathcal{E}^2$$

$$E^{(2)} = -\frac{9}{4}a^3\mathcal{E}^2$$

$$\chi = -\frac{\partial^2 E^{(2)}}{\partial\mathcal{E}^2} = \frac{9a^3}{2}$$

Solution. еще одно, давнее

как энергии -поскольку $\frac{\partial E_0}{\partial \varepsilon} = \langle \frac{\partial \hat{V}}{\partial \mathcal{E}} \rangle = -\langle \hat{d}(\mathcal{E}) \rangle = -\chi \mathcal{E} \to \delta E_0 = -\frac{1}{2}\chi \mathcal{E}^2$. Именно второй поправкой к уровню энергии мы и займёмся.

Для конкретности, мы будем исследовать поляризуемость основного состояния в одномерной мелкой яме $\hat{H}_0 = \hat{p}^2/(2m) - (\kappa/m)\cdot\delta(x)$, в которой параметр κ связан с энергией связанного состояния в этой яме как $E_0 = \kappa^2/(2m)$ и в таком случае, оператор дипольного момента - это просто $\hat{d} = -e\hat{x}$.

Волновая функция связанного состояния мелкой ямы $\langle x|\psi_0\rangle = \sqrt{\kappa}e^{-\kappa|x|}$ является чётной; возмущение же -нечётное.

Поэтому первый порядок теории возмущений $E_0^{(1)} = \langle\psi_0|\hat{V}|\psi_0\rangle \equiv 0$ - что неудивительно (если сдвиг энергии линеен но полю, то это означает, что исходно система обладает дипольным моментом $\frac{\partial E_0}{\partial \varepsilon} = d = \text{const}$).

Волновые функции непрерывного спектра также удобно классифицировать по чётности - имеются чётные функции $\psi_k^{(+)}$ и нечётные функции $\psi_k^{(-)}$

$$\langle x|\psi_k^{(-)}\rangle = \sin kx, \quad \langle x|\psi_k^{(+)}\rangle = \cos\left(k|x| + \varphi_k\right), \quad E_k = \frac{k^2}{2m}$$

Такой вид волновых функций обусловлен следующим соображением.

Нечётная функция в нуле обращается в ноль, из-за чего она эффективно не чувствуется дельта-яму - поэтому волновая функция нечётного состояния совпадает с волновой функцией свободного движения.

Чётная же функция обязана испытывать излом шри $x = 0$, что обуславливает наличие фазового сдвига φ_k, как-то зависящего от параметров задачи.

Явный вид фазового сдвига, тем не менее, нам не нужен - ведь, опять-таки, из соображений чётности, виртуальные переходы будут только в нечётные состояния непрерывного спектра (только для них матричный элемент возмущения V_{0k} отличен от нуля).

Поправка второго порядка тогда имеет виу:

$$E_0^{(2)} = \int d\nu_k \frac{|V_{k0}|^2}{E_0^{(0)} - E_k^{(0)}}$$

Плотность состояний непрерывного спектра $d\nu_k$ находится из нормировки волновых функций - несложно убедиться, что $\langle\psi_{k'}^{(+)}|\psi_k^{(+)}\rangle = \pi\delta\left(k - k'\right)$, поэтому $d\nu_k = \frac{dk}{\pi}$.

Величины V_{k0} вычисляются по определению:

$$V_{k0} = \int\limits_{-\infty}^{\infty} dx \sin kx \cdot e\mathcal{E}x \cdot \sqrt{\kappa}e^{-\kappa|x|} = -2e\mathcal{E}\sqrt{\kappa}\partial_k \operatorname{Re}\int\limits_0^{\infty} dx e^{ikx-\kappa x} = 4e\mathcal{E}\frac{k\kappa^{3/2}}{\left(\kappa^2+k^2\right)^2}$$

Теперь посчитаем $E_0^{(2)}$, Подставим $k = \kappa x$, получаем:

$$E_0^{(2)} = -\frac{8me^2\mathcal{E}^2}{\pi\kappa^4}\int\limits_0^{\infty}\frac{x^2dx}{\left(1+x^2\right)^5} = -\frac{5}{32}\frac{e^2\mathcal{E}^2}{mE_0^2}$$

и в итоге:

$$\chi = -\frac{\partial^2 E_0}{\partial\mathcal{E}^2} = \frac{5}{16}\frac{e^2}{mE_0^2}$$

ПТФ-7.з4. Суперсимметричная квантовая механика

Рассмотрите гармонический осциллятор для частицы массы $m = 1$ с частотой $\omega = 1$, гамильтониан которого имеет вид $\hat{H} = \frac{1}{2}(\hat{p}^2 + \hat{x}^2 - 1)$, и основное состояние имеет нулевую энергию $E_0 = 0$. Помимо этого, имеется ангармонизм *очень* специального вида $V(x) = gx(1-x^2) + \frac{1}{2}g^2x^4$; безразмерный параметр $g \ll 1$. Требуется исследовать сдвиг энергии основного состояния с точки зрения теории возмущений.

• Найдите поправку $O(g^2)$ к энергии основного состояния осциллятора.

• Полученный ответ должен вас натолкнуть на мысль, что нужно считать старшие порядки ТВ (если нет, то перепроверьте). Удобнее всего это делать в координатном базисе, выписывая явно дифференциальные уравнения на поправки к волновым функциям. Выпишите такое уравнение на поправки $O(g)$ и $O(g^2)$, и решите их явно.

• Проделайте это в *произвольном* порядке теории возмущений, выпишите явно поправку произвольного порядка к волновой функции $\psi_0^{(n)}(x)$ и $E_0^{(n)}$. Просуммируйте весь ряд теории возмущений, и убедитесь, что вы, в действительности, нашли *точное решение* соответствующего

уравнения Шрёдингера. Расстройтесь, потому что это решение никак не позволяет ответить на вопрос, каков же в действительности сдвиг энергии основного состояния δE_0.

• Очевидно, что поправка к энергии основного состояния всё-таки имеется – но она *непертурбативна*, для неё невозможно построить асимптотический ряд по степеням малого параметра g. Не смотря на это, теорией возмущений всё-таки можно пользоваться для приближения основного состояния, просто использовать для этого *полный ряд* теории возмущений незаконно. Используя критерии применимости теории возмущений, определите максимальный порядок n^*, до которого результату ещё можно верить.

• Погрешность асимптотического ряда для волновой функции – то есть отличие истинной волновой функции от вычисленной при помощи ряда теории возмущений – может быть оценена как член ряда теории возмущений с порядковым номером n^*. Оцените с экспоненциальной точностью квадрат нормы $\langle\delta\psi|\delta\psi\rangle$ этой погрешности; это даст также и оценку отличия энергии основного состояния от нуля.

Указание: хотя возмущение и содержит линейный член по x, с точки зрения вычислений оказывается удобно не сдвигать центр осциллятора.

Solution.

• Обозначим возмущения $V_1 = gx(1-x^2)$, $V_2(x) = \frac{g^2x^4}{2}$. Основное состояние осциллятора: $\psi^{(0)}(x) = \frac{e^{-\frac{x^2}{2}}}{\sqrt[4]{\pi}}$.

Рассмотрим 1 порядок теории возмущений:

$$(\hat{H}+\hat{V}_1)(|\psi^{(0)}\rangle + |\psi^{(1)}\rangle) = (E^{(0)}+E^{(1)})(|\psi^{(0)}\rangle + |\psi^{(1)}\rangle)$$

Поскольку $E^{(0)} = E_0 = 0$, то $\hat{H}|\psi^{(0)}\rangle = 0$ и

$$\hat{V}_1|\psi^{(0)}\rangle + \hat{H}|\psi^{(1)}\rangle = E^{(1)}|\psi^{(0)}\rangle$$

Домножив скалярно на $\langle\psi^{(0)}|$, получим

$$\langle\psi^{(0)}|\hat{V}_1|\psi^{(0)}\rangle + \langle\psi^{(0)}|\hat{H}|\psi^{(1)}\rangle = \langle\psi^{(0)}|E^{(1)}|\psi^{(0)}\rangle$$

$$E^{(1)} = \langle\psi^{(0)}|\hat{V}_1|\psi^{(0)}\rangle$$

Из нечётности $\hat{V}_1$ получим

$$E^{(1)} = 0$$

Полученный ответ наталкивает на мысль перейти ко 2 пункту.

• 1 порядок теории возмущений:

$$\hat{H}\psi^{(1)} + \hat{V}^{(1)}\psi^{(0)} = 0$$

$$\frac{1}{2}\left(-\frac{\partial^2}{\partial x^2} + x^2 - 1\right)\psi^{(1)}(x) + gx(1-x^2)\frac{e^{-\frac{x^2}{2}}}{\sqrt[4]{\pi}} = 0$$

$$\psi^{(1)}(x) = e^{-\frac{x^2}{2}}f(x)$$

$$\left(fe^{-\frac{x^2}{2}}\right)'' = \left(-xfe^{-\frac{x^2}{2}} + f'e^{-\frac{x^2}{2}}\right)' = e^{-\frac{x^2}{2}}((x^2-1)f(x) - 2xf'(x) + f''(x))$$

$$2xf'(x) - f''(x) + \frac{2gx(1-x^2)}{\sqrt[4]{\pi}} = 0$$

Ищем $f(x)$ в виде:

$$f(x) = Bx + Cx^2 + Dx^3$$

$$2x(B + 2Cx + 3Dx^2) - 2C - 6Dx + \frac{2gx(1-x^2)}{\sqrt[4]{\pi}} = 0$$

$$\begin{cases} C = 0, \\ 2B - 6D + \frac{2g}{\sqrt[4]{\pi}} = 0, \\ 6D - \frac{2g}{\sqrt[4]{\pi}} = 0. \end{cases}$$

$$B = C = 0, \quad D = \frac{g}{3\sqrt[4]{\pi}}$$

$$f(x) = \frac{gx^3}{3\sqrt[4]{\pi}}$$

$$\psi^{(1)}(x) = \frac{gx^3 e^{-\frac{x^2}{2}}}{3\sqrt[4]{\pi}}$$

Рассмотрим 2 порядок теории возмущений:

$$(\hat{H} + \hat{V}_1 + \hat{V}_2)(|\psi^{(0)}\rangle + |\psi^{(1)}\rangle + |\psi^{(2)}\rangle) = (E^{(0)} + E^{(1)} + E^{(2)})(|\psi^{(0)}\rangle + |\psi^{(1)}\rangle + |\psi^{(2)}\rangle)$$

$$\hat{H}|\psi^{(2)}\rangle + \hat{V}_1|\psi^{(1)}\rangle + \hat{V}_2|\psi^{(0)}\rangle = E^{(0)}|\psi^{(2)}\rangle + E^{(1)}|\psi^{(1)}\rangle + E^{(2)}|\psi^{(0)}\rangle$$

Домножим скалярно на $\langle\psi^{(0)}|$ и воспользуемся тем, что $E^{(0)} = 0$:

$$\langle\psi^{(0)}|\hat{V}_1|\psi^{(1)}\rangle + \langle\psi^{(0)}|\hat{V}_2|\psi^{(0)}\rangle = E^{(2)}$$

$$E^{(2)} = \int\limits_{-\infty}^{\infty} \frac{e^{-\frac{x^2}{2}}}{\sqrt[4]{\pi}} \frac{gx^3 e^{-\frac{x^2}{2}}}{3\sqrt[4]{\pi}} gx(1-x^2)dx + \int\limits_{-\infty}^{\infty} \frac{e^{-x^2}}{\sqrt{\pi}} \frac{g^2x^4}{2} dx = -\frac{3g^2}{8} + \frac{3g^2}{8} = 0$$

$$E^{(2)} = 0$$

$$\hat{H}^{(0)}\psi^{(2)} + \hat{V}^{(1)}\psi^{(1)} + \hat{V}^{(2)}\psi^{(0)} = 0$$

$$\frac{1}{2}\left(-\frac{\partial^2}{\partial x^2} + x^2\right)\psi^{(2)} + gx(1-x^2)\frac{gx^3}{3\sqrt[4]{\pi}} e^{-\frac{x^2}{2}} + \frac{g^2x^4 e^{-\frac{x^2}{2}}}{2\sqrt[4]{\pi}} = 0$$

Решая ДУ аналогично предыдущему, получим

$$\psi^{(2)} = \frac{g^2x^6}{18\sqrt[4]{\pi}} e^{-\frac{x^2}{2}}$$

- Рассмотрим произвольный n-й порядок теории возмущений:

$$\hat{H}|\psi^{(n)}\rangle + \hat{V}_1|\psi^{(n-1)}\rangle + \hat{V}_2|\psi^{(n-2)}\rangle = E^{(0)}|\psi^{(n)}\rangle + E^{(1)}|\psi^{(n-1)}\rangle + ... + E^{(n)}|\psi^{(0)}\rangle$$

Домножим скалярно на $\langle\psi^{(0)}|$ и воспользуемся тем, что $E^{(0)} = 0$:

$$E^{(n)} = \langle\psi^{(0)}|\hat{V}_1|\psi^{(n-1)}\rangle + \langle\psi^{(0)}|\hat{V}_2|\psi^{(n-2)}\rangle$$

Докажем по индукции одновременно 2 утверждения: $E^{(n)} = 0$ и $\psi^{(n)} = \frac{g^n x^{3n}}{\sqrt[4]{\pi} 3^n n!} e^{-\frac{x^2}{2}}$. Пусть это верно $\forall k \leq n-1$. Тогда

$$E^{(n)} = \int\limits_{-\infty}^{\infty} \frac{e^{-\frac{x^2}{2}}}{\sqrt[4]{\pi}} \frac{g^n x^{3(n-1)}}{\sqrt[4]{\pi} 3^{n-1}(n-1)!} e^{-\frac{x^2}{2}} gx(1-x^2)dx + \int\limits_{-\infty}^{\infty} \frac{e^{-\frac{x^2}{2}}}{\sqrt[4]{\pi}} \frac{g^{n-2} x^{3(n-2)}}{\sqrt[4]{\pi} 3^{n-2}(n-2)!} e^{-\frac{x^2}{2}} \frac{g^2x^4}{2} dx =$$

$$= -\frac{3^{2-n}(1+(-1)^{3n}) g^n \Gamma(\frac{3n}{2} - \frac{1}{2})}{4\sqrt{\pi}(n-2)!} + \frac{3^{2-n}(1+(-1)^{3n}) g^n \Gamma(\frac{3n}{2} - \frac{1}{2})}{4\sqrt{\pi}(n-2)!} = 0$$

$$E^{(n)} = 0$$

Теперь проверим, что будет выполняться:

$$\hat{H}\psi^{(n)} + \hat{V}^{(1)}\psi^{(n-1)} + \hat{V}^{(2)}\psi^{(n-2)} = 0$$

$$\frac{1}{2}\left(-\frac{\partial^2}{\partial x^2} + x^2\right)\frac{g^n x^{3n}}{\sqrt[4]{\pi} 3^n n!} e^{-\frac{x^2}{2}} + gx(1 - x^2)\frac{g^{n-1} x^{3(n-1)}}{\sqrt[4]{\pi} 3^{n-1}(n-1)!} e^{-\frac{x^2}{2}} + \frac{g^2x^4}{2}\frac{g^{n-2} x^{3(n-2)}}{\sqrt[4]{\pi} 3^{n-2}(n-2)!} e^{-\frac{x^2}{2}} = 0$$

Таким образом, поправка произвольного порядка к волновой функции:

$$\psi^{(n)} = \frac{g^n x^{3n}}{\sqrt[4]{\pi} 3^n n!} e^{-\frac{x^2}{2}}$$

Просуммируем ряд возмущений:

$$\psi(x) = \sum_{n=0}^{\infty} \frac{g^n x^{3n}}{\sqrt[4]{\pi} 3^n n!} e^{-\frac{x^2}{2}} = \frac{e^{-\frac{x^2}{2}}}{\sqrt[4]{\pi}} \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{gx^3}{3}\right)^n = \frac{\exp\left(g\frac{x^3}{3} - \frac{x^2}{2}\right)}{\sqrt[4]{\pi}}$$

Проверим, что это точное решение уравнения Шрёдингера:

$$\left(\frac{1}{2}\left(-\frac{\partial^2}{\partial x^2}+x^2-1\right)+gx(1-x^2)+\frac{g^2x^4}{2}\right)\psi(x)=E\psi(x)$$

$$\frac{1}{2}\left(-\frac{\partial^2}{\partial x^2}+x^2-1\right)\psi(x)=-\frac{gx(2-2x^2+gx^3)}{2\sqrt[4]{\pi}}\exp\left(g\frac{x^3}{3}-\frac{x^2}{2}\right)$$

$$\left(\frac{1}{2}\left(-\frac{\partial^2}{\partial x^2}+x^2-1\right)+gx(1-x^2)+\frac{g^2x^4}{2}\right)\psi(x)=0$$

Таким образом, точное решение уравнения Шрёдингера:

$$\psi(x)=\frac{\exp\left(g\frac{x^3}{3}-\frac{x^2}{2}\right)}{\sqrt[4]{\pi}}$$

Расстраиваемся, поскольку это решение никак не позволяет ответить на вопрос, какой сдвиг энергии $\delta E_0=\sum\limits_{n=0}^{\infty}E^{(n)}=0$.

- Критерий применимости теории возмущений:

$$\langle\psi^{(n)}|\psi^{(n)}\rangle\gg\langle\psi^{(n+1)}|\psi^{(n+1)}\rangle$$

$$\langle\psi^{(n)}|\psi^{(n)}\rangle=\int\limits_{-\infty}^{\infty}\frac{g^{2n}x^{6n}}{\sqrt{\pi}3^{2n}(n!)^2}e^{-x^2}dx=\frac{g^{2n}\Gamma(3n+\frac{1}{2})}{\sqrt{\pi}3^{2n}\Gamma(n+1)^2}=\frac{g^{2n}(6n)!}{2^{6n}3^{2n}(n!)^2(3n)!}$$

При больших n воспользуемся формулой Стирлинга:

$$n!\approx\sqrt{2\pi n}\left(\frac{n}{e}\right)^n$$

$$\langle\psi^{(n)}|\psi^{(n)}\rangle\sim\frac{g^{2n}\sqrt{12\pi n}(6n)^{6n}}{2^{6n}3^{2n}2\pi n^{2n+1}\sqrt{6\pi n}(3n)^{3n}}=\frac{3^ng^{2n}n^{n-1}}{\sqrt{2}\pi}$$

$$\frac{\langle\psi^{(n+1)}|\psi^{(n+1)}\rangle}{\langle\psi^{(n)}|\psi^{(n)}\rangle}=\frac{3g^2(n+1)^n}{n^{n-1}}\approx3g^2n\ll1$$

$$n^*\gg\frac{1}{3g^2}$$

Например, можно взять другую степень g:

$$n^*=\frac{1}{3g}$$

- Подставим n^*:

$$\langle\delta\psi|\delta\psi\rangle=\langle\psi^{(n^*)}|\psi^{(n^*)}\rangle=\frac{3^{n^*}g^{2n^*}(n^*)^{n^*-1}}{\sqrt{2}\pi}$$

Смещение энергии в колодце при $\mathrm{V(x)}=\frac{\mathrm{V_0}}{a^2}(a-\mathrm{x})\mathrm{x}$ (???)

Solution.

Для частицы, находящейся в бесконечно глубокой потенциальной яме шириной, $a(0<x<a)$ найти в первом приближении теории возмущений смещение энергетических уровней под воздействием возмущения вида

$$\mathrm{V(x)}=\frac{\mathrm{V_0}}{a^2}(a-\mathrm{x})\mathrm{x}.$$

Волновые функции для координаты в яме: $\varphi_n(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{\pi n}{a}x\right)$, в других координатах 0.

По первому порядку нестационарной теории возмущений $\Delta E=V_{nn}=\frac{V_0}{a^3}\int\limits_0^a(ax-x^2)\left(a-\cos\left(\frac{2\pi nx}{a}\right)\right)dx$.

Разбиваем интеграл на 4, один равен нулю, остальные дают:

$$\Delta E=\frac{V_0}{a^3}\left(\frac{a^3}{2}-\frac{a^3}{3}-\frac{a^3}{2(\pi n)^2}\right)=V_0\left(\frac{1}{6}-\frac{1}{2(\pi n)^2}\right).$$

Б-2.8.1 Поправки к осциллятору при $\hat{\mathrm{V}} = \alpha x$ и $\hat{\mathrm{V}} = Ax^3 + Bx^4$

Найти с помощью теории возмущений поправки к уровням энергии линейного гармонического осциллятора, возмущенного полем вида:

а) однородное поле $\hat{\mathrm{V}} = \alpha x$;

б) $\hat{\mathrm{V}} = Ax^3 + Bx^4$.

Поправка к энергии осциллятора при $V = \alpha x$.

Операторы координаты в представлении операторов рождения и уничтожения равен $x = \frac{x_0}{\sqrt{2}}\left(a^\dagger + a\right)$, где $x_0 = \sqrt{\frac{\hbar}{m\omega}}$.

Поправка первого порядка ϵ_1 по теории возмущений для $V = \alpha x$ равна нулю:

$$\epsilon_1 = V_{nn} = \frac{\alpha x_0}{\sqrt{2}}\langle n|a^\dagger + a|n\rangle = 0,$$

ведь $\langle n|a^\dagger|n\rangle \sim \langle n|n+1\rangle = 0$, $\langle n|a|n\rangle \sim \langle n|n-1\rangle = 0$.

Вычислим поправку второго порядка по $\epsilon_2 = \sum\limits_{k\neq n} \frac{|V_{kn}|^2}{E_n - E_k}$, в ней

$$V_{kn} \equiv \langle k|V|n\rangle = \frac{\alpha x_0}{\sqrt{2}}\langle k|a^\dagger + a|n\rangle = \frac{\alpha x_0}{\sqrt{2}}\left[\sqrt{n+1}\delta_{k,n+1} + \sqrt{n}\delta_{k,n-1}\right].$$

То есть у нас $k = \{n+1, n-1\}$. Из того, что $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$, знаменатели двух членов суммы равны $\hbar\omega$ и -$\hbar\omega$. В итоге

$$\epsilon_2 = \sum_{k\neq n}\frac{|V_{kn}|^2}{E_n - E_k} = \frac{\alpha^2 x_0^2}{2}\left[-\frac{n+1}{\hbar\omega} + \frac{n}{\hbar\omega}\right] = -\frac{\alpha^2 x_0^2}{2\hbar\omega} = -\frac{\alpha^2}{2m\omega^2}$$

(???? что за классическая интерпретация этой поправки????)

Как видим, поправка оказалась не зависящей от постоянной Планка, поэтому она имеет классическую интерпретацию. Действительно, если бы мы записали полный гамильтониан с учетом возмущения (1) и выделили бы полный квадрат, мы бы получили, что все уровни энергии сдвинулись на одинаковую величину, совпадающую с полученной по теории возмущений, но при этом и изменилось бы равновесное значение координаты осциллятора. Для нахождения смещения положения равновесия осциллятора по теории возмущений необходимо знать «поправленные векторы состояния.

Поправка к энергии осциллятора при $V = \alpha x^3$.

Для поправки первого порядка $\epsilon_1 = V_{nn} = \frac{\alpha x_0^3}{2\sqrt{2}}\langle n|\left(a^\dagger + a\right)^3|n\rangle$ преобразуем $\left(a^\dagger + a\right)^3$:

$$\left(a^\dagger + a\right)^2 = \left(a^\dagger + a\right)\left(a^\dagger + a\right) = a^\dagger a^\dagger + aa + aa^\dagger + a^\dagger a = a^\dagger a^\dagger + aa + 2N + 1.$$

Тут учтено, что $\left[a, a^\dagger\right] = 1$, $N = a^\dagger a$ - оператор числа квантов: $N|n\rangle = n|n\rangle$, $Na \neq aN$. Получаем оператор

$$\left(a^\dagger + a\right)^3 = a^\dagger a^\dagger a^\dagger + aaa + (N+1)a^\dagger + a^\dagger(2N+1) + Na + a(2N+1),$$

тогда поправка:

$$\epsilon_1 = V_{nn} = \frac{\alpha x_0^3}{2\sqrt{2}}\langle n|\left(a^\dagger + a\right)^3|n\rangle \sim 0 + 0 + 0 + 0 + 0 + 0 = 0.$$

Для поправки второго порядка $\epsilon_2 = \sum\limits_{k\neq n}\frac{|V_{kn}|^2}{E_n - E_k}$, где $V_{kn} = \frac{\alpha x_0^3}{2\sqrt{2}}\langle k|\left(a^\dagger + a\right)^3|n\rangle$ посчитаем

$$\begin{aligned}
\langle k|a^\dagger a^\dagger a^\dagger|n\rangle &= ((n+1)(n+2)(n+3))^{1/2}\delta_{k,n+3}\\
\langle k|aaa|n\rangle &= (n(n-1)(n-2))^{1/2}\delta_{k,n-3}\\
\langle k|(N+1)a^\dagger + a^\dagger(2N+1)|n\rangle &= \sqrt{n+1}(n+2+2n+1)\langle k|n+1\rangle = 3(n+1)^{3/2}\delta_{k,n+1}\\
\langle k|Na + a(2N+1)|n\rangle &= \sqrt{n}(n-1+2n+1)\langle k|n-1\rangle = 3n^{3/2}\delta_{k,n-1}
\end{aligned}$$

Получим:

$$\begin{aligned}
\epsilon_2 &= \frac{\alpha^2 x_0^6}{8\hbar\omega}\left[\frac{9n^3}{n-(n-1)} + \frac{9(n+1)^3}{n-(n+1)} + \frac{(n+1)(n+2)(n+3)}{n-(n+3)} + \frac{n(n-1)(n-2)}{n-(n-3)}\right] =\\
&= \frac{\alpha^2 x_0^6}{8\hbar\omega}\left[-27n^2 - 27n - 9 - 3n^2 - 3n - 2\right] =\\
&= -\alpha^2\left(\frac{\hbar}{m\omega}\right)^3\frac{15}{4\hbar\omega}\left[n^2 + n + \frac{11}{30}\right]
\end{aligned}$$

Поправка к энергии осциллятора при $V = \beta x^4$.

Для поправки первого порядка $\epsilon_1' = \langle n|V|n\rangle = \frac{\beta x_0^4}{4}\langle n|\left(a^\dagger + a\right)^4|n\rangle$ найдем:

$$\begin{aligned}\left(a^\dagger + a\right)^4 &= \left(a^\dagger a^\dagger + aa + 2N + 1\right)\left(a^\dagger a^\dagger + aa + 2N + 1\right) = \\ &= a^\dagger a^\dagger a^\dagger a^\dagger + aaaa + a^\dagger N a + a^\dagger a^\dagger (2N+1) + \\ &\quad + a(N+1)a^\dagger + aa(2N+1) + (2N+1)a^\dagger a^\dagger + (2N+1)aa + (2N+1)^2.\end{aligned}$$

Ненулевые останутся для первого порядка теории возмущений только члены, в которых одинаковое количество a и $a^\dagger$, подставим их:

$$\epsilon_1' = \frac{\beta x_0^4}{4}\langle n|\left(a^\dagger + a\right)^4|n\rangle = \frac{\beta x_0^4}{4}\left[n(n-1) + (n+1)(n+2) + (2n+1)^2\right] = \frac{3\beta x_0^4}{2}\left(n^2 + n + \frac{1}{2}\right)$$

Для поправки при $\hat{\mathrm{V}} = Ax^3 + Bx^4$ имеем сумму:

$$\Delta\epsilon = \frac{3}{2}\beta\left(\frac{\hbar}{m\omega}\right)^2\left[n^2 + n + \frac{1}{2}\right] - \alpha^2\left(\frac{\hbar}{m\omega}\right)^3\frac{15}{4\hbar\omega}\left[n^2 + n + \frac{11}{30}\right]$$

(??? почему так можно складывать - зависший вопрос в теории, пока забил.)

(тут мб когда-то посчитаю поправку 2го порядка. Так типично мало кто делает, потому что куча возни с операторами, так что пока что я забил. когда-то мб вернусь к этому, пока тут нерешенная часть задачи.)

Поправка к энергии осциллятора при $V = \alpha x$, если работать через функции Эрмита (!??!??!?)

(??? что если не переходить к оператором рождения и уничтожения, задача так вообще решается??)

Б-2.8.2 Поправки к векторам состояния осциллятора в $\hat{\mathrm{V}} = \alpha\hat{x}$

Найти поправки к уровням энергии и векторам состояния одномерного гармонического осциллятора, помещенного в однородное поле $\hat{\mathrm{V}} = \alpha\hat{x} = \frac{\alpha x_0}{\sqrt{2}}(\hat{a}^+ + \hat{a})$, где α - некоторая константа взаимодействия.

Solution.

Поправки первого порядка к векторам состояний находим по типичной формуле $|\psi_n^{(1)}\rangle = \sum\limits_{k\neq n}\frac{\langle k|\hat{\mathrm{V}}|n\rangle}{E_n^{(0)} - E_k^{(0)}}|\psi_k^{(0)}\rangle$. Уже найдено $V_{kn} = \frac{\alpha x_0}{\sqrt{2}}\langle k|a^\dagger + a|n\rangle = \frac{\alpha x_0}{\sqrt{2}}\left[\sqrt{n+1}\delta_{k,n+1} + \sqrt{n}\delta_{k,n-1}\right]$, поэтому

$$|\psi_n\rangle = |n\rangle + |\psi_n^{(1)}\rangle = |n\rangle + \frac{\alpha x_0}{\sqrt{2}\hbar\omega}(\sqrt{n}|n-1\rangle - \sqrt{(n+1)}|n+1\rangle).$$

Кстати, среднее значение оператора координаты $\hat{x}$ для состояния $|\psi_n\rangle$ с учетом поправок первого приближения:

$$\begin{aligned}\langle\psi_n|\hat{x}|\psi_n\rangle &= \frac{x_0}{\sqrt{2}}\left(\langle n|\left(\hat{a} + \hat{a}^+\right)|\psi_n^{(1)}\rangle + \langle\psi_n^{(1)}|\left(\hat{a} + \hat{a}^+\right)|n\rangle\right) = \\ &= \frac{\alpha x_0^2}{\hbar\omega}\left(\sqrt{n}\langle n|\hat{a}^+|n-1\rangle - \sqrt{(n+1)}\langle n|\hat{a}|n+1\rangle\right) = -\frac{\alpha}{m\omega^2}.\end{aligned}$$

Полученный результат в точности совпадает с тем, который получается в результате выделения в гамильтониане полного квадрата (????? пока верю, потом проделаю, проверю!!!!).

(?? а с учетом поправок второго приближения что можно сказать???)

Б-2.8.3 Расщепление 1го уровня энергии и правильные волновые функции функции 3D осциллятора при $\hat{\mathrm{V}} = \alpha xy$

Определить расщепление первого возбужденного уровня энергии трехмерного изотропного гармонического осциллятора и найти правильные векторы нулевого приближения при воздействии на него возмущения вида $\hat{\mathrm{V}} = \alpha xy$.

Solution.

Состояния 3D изотропного осциллятора определяются 3-мя квантовыми числами $|n_1, n_2, n_3\rangle$. Первый возбужденный уровень энергии трехкратно вырожден.

Обозначим состояния следующим образом:

$$|1\rangle = |1,0,0\rangle, \quad |2\rangle = |0,1,0\rangle, \quad |3\rangle = |0,0,1\rangle.$$

Оператор возмущения выразим через повышающие и понижающие операторы

$$\hat{\mathrm{V}} = \frac{1}{2}\alpha x_0^2 \left(\hat{a}_x^+ + \hat{a}_x\right)\left(\hat{a}_y^+ + \hat{a}_y\right),$$

где ω - частота осциллятора, $x_0 = \sqrt{\hbar/(m\omega)}$.

Легко видеть, что все диагональные матричные элементы оператора возмущения равны нулю, а отличны от нуля только два недиагональных:

$$V_{11} = V_{22} = V_{33} = V_{13} = V_{23} = 0, \quad V_{12} = V_{21} = \frac{1}{2}\alpha x_0^2.$$

Таким образом, получаем, что состояние $|3\rangle = |0,0,1\rangle$ - правильное и имеет энергию, совпадающую с энергией первого возбужденного уровня невозмущенного осциллятора. Два других правильных состояния определяются линейными комбинациями

$$|\pm\Delta\rangle = \frac{1}{\sqrt{2}}(|1,0,0\rangle \pm |0,1,0\rangle)$$

и поправки к невозмущенному уровню энергии $\Delta E \pm \alpha x_0^2/2$.

Расщепление 1го уровня энергии 2d осциллятора при $V = \alpha x^3 y^3$

Найти расщепление первого возбужденного уровня энергии плоского гармонического осциллятора под действием возмущения вида $V = \alpha x^3 y^3$ (плоскость x, y-плоскость колебаний) в первом порядке теории возмущений.

Solution.

(!! укажу потом, что важно нормально занумеровать, в каком состоянии частица сколько энергии дает. в этом самая основная путаница, дальше уже их операторами рождения и уничтожения переводим одно в другое. собственно, все тут однообразно решается.)

Первый уровень двумерного осциллятора двукратно вырожден, его энергия $E = \hbar\omega(0+1/2) + \hbar\omega(1+1/2) = 2\hbar\omega$.

Для секулярного уравнения расписываем оператор возмущения выразим через повышающие и понижающие операторы

$$\hat{\mathrm{V}} = \frac{1}{8}\alpha x_0^6 \left(\hat{a}_x^+ + \hat{a}_x\right)^3 \left(\hat{a}_y^+ + \hat{a}_y\right)^3,$$

дальше их в полиномы раскладываем по типичным формулам, действуем на состояния, диагональные элементы дают ноль, кросдиагональные равны $\frac{9\alpha x_0^6}{8}$, из секулярного уравнения получаем, что поправка $\Delta E = +\frac{9\alpha x_0^6}{8}$ и $\Delta E = -\frac{9\alpha x_0^6}{8}$. В итоге $E_1' = 2\hbar\omega \pm \frac{9\alpha\hbar^3}{8m^3\omega^3}$.

Б-2.8.4 Уравнение на эффективный оператор возмущения (???)

Предположим, что в случае вырожденного энергетического спектра все матричные элементы оператора возмущения для состояний, относящихся к данному уровню энергии $E_n^{(0)}$, равны нулю.

Показать, что при этом поправки к уровню энергии и правильные векторы нулевого приближения можно найти из уравнения (??) для эффективного оператора возмущения

$$\hat{\mathrm{V}}^{\mathrm{eff}} = \hat{\mathrm{V}} \sum_{k,\nu} \frac{|\psi_{k\nu}^{(0)}\rangle\langle\psi_{k\nu}^{(0)}|}{E_n^{(0)} - E_k^{(0)}} \hat{\mathrm{V}},$$

которым можно пользоваться только при действии на состояния, относящиеся к уровню энергии $E_n^{(0)}$.

Solution.

(?? вообще не знаю такое ещё. какая-то тупая теория.)

2.8.4. Поскольку в рассматриваемом случае все матричные элементы оператора возмущения для состояний, относящихся к вырожденному уровню энергии $E_n^{(0)}$, равны нулю, то общий вид вектора состояния с учетом первого приближения теории возмущений определяется стандартным образом в соответствии с (II.40):

$$|\psi_{n\mu}\rangle \simeq |\psi_{n\mu}^{(0)}\rangle + \sum_{k,\nu}{}' \frac{\langle k\nu|\hat{\mathrm{V}}|n\mu\rangle}{E_n^{(0)} - E_k^{(0)}} |\psi_{k\nu}^{(0)}\rangle,$$

где штрих означает отсутствие в сумме слагаемых с $n = k, \mu = \nu$. Составим теперь из состояний (1), относящихся к одному и тому же уровню энергии $E_n^{(0)}$, линейные комбинации

$$|\Phi_{n\alpha}\rangle = \sum_{\mu} C_\mu^\alpha |\psi_{n\mu}\rangle$$

и подставим их в уравнение Шредингера:

$$\left(\hat{\mathrm{H}}^{(0)} + \hat{\mathrm{V}}\right) |\Phi_{n\alpha}\rangle = E_{n\alpha} |\Phi_{n\alpha}\rangle.$$

Теперь мы можем получить систему алгебраических уравнений, аналогичную системе (II.41), из которой определяются поправки второго порядка к уровню энергии и, соответственно, коэффициенты линейных комбинаций (2), дающих правильные векторы первого приближения:

$$\sum_{\beta} \left(\sum_{k,\nu}{}' \langle n\alpha|\hat{\mathrm{V}}|k\nu\rangle \frac{\langle k\nu|\hat{\mathrm{V}}|n\beta\rangle}{E_n^{(0)} - E_k^{(0)}} - \varepsilon\delta_{\alpha\beta} \right) C_\beta = 0.$$

Уравнение формально сводится к стандартному (см. (II.41)), если ввести оператор возмущения $\hat{\mathrm{V}}^{\mathrm{elf}}$.

17.1.2 Problems about Time-Independent PT 2

Б-2.8.5 Поправка ко 2му уровню 3d осциллятора при $\hat{\mathrm{V}} = \beta xz$

Определить поправки ко второму возбужденному уровню энергии трехмерного изотропного гармонического осциллятора и правильные векторы нулевого приближения при воздействии на него возмущения вида $\hat{\mathrm{V}} = \beta xz$.

Solution.

2.8.5. Второй возбужденный уровень трехмерного изотропного гармонического осциллятора шестикратно вырожден. Обозначим состояния так же, как и в задаче 2.8.3:

$$\begin{array}{lll} |1\rangle = |2,0,0\rangle, & |2\rangle = |0,2,0\rangle, & |3\rangle = |0,0,2\rangle, \\ |4\rangle = |1,1,0\rangle, & |5\rangle = |1,0,1\rangle, & |6\rangle = |0,1,1\rangle. \end{array}$$

Для состояний $|4\rangle - |6\rangle$ отличны от нуля только диагональные матричные элементы эффективного оператора возмущения $\hat{\mathrm{V}}^{\mathrm{eff}}$ задачи 2.8.4. Таким образом, получаем трехкратно вырожденный уровень, смещенный на величину $-\Delta$, где

$$\Delta = \frac{\beta^2\hbar}{4m^2\omega_0^3},$$

которому соответствуют три произвольные линейно независимые комбинации состояний $|4\rangle - |6\rangle$. При действии оператора возмущения $\hat{\mathrm{V}}^{\mathrm{eff}}$ состояния $|1\rangle - |3\rangle$ «смешиваются», поскольку отличны от нуля как диагональные, так и недиагональные матричные элементы:

$$V_{11} = V_{22} = V_{33} = -\frac{1}{2}\Delta, \quad V_{12} = V_{23} = V_{13} = -\Delta.$$

Таким образом, получаем секулярное уравнение третьей степени, корни которого, однако, легко находятся и равны

$$\varepsilon_{1,2} = \Delta, \quad \varepsilon_3 = -\frac{5}{8}\Delta.$$

Правильный вектор состояния для поправки ε_3 равен

$$|\varepsilon_3\rangle = \frac{1}{\sqrt{3}}(|2,0,0\rangle + |0,2,0\rangle + |0,0,2\rangle).$$

Для двукратно вырожденного уровня $\varepsilon_{1.2}$ правильными будут линейные комбинации, ортогональные вектору состояния $|\varepsilon_3\rangle$ и имеющие вид

$$|I\rangle = \sqrt{\frac{2}{3}}\left(\frac{1}{2}(|2,0,0\rangle + |0,2,0\rangle) - |0,0,2\rangle\right).$$
$$|II\rangle = \sqrt{\frac{2}{3}}\left(\frac{1}{2}(|2,0,0\rangle + |0,0,2\rangle) - |0,2,0\rangle\right).$$

Как видим, шестикратно вырожденный уровень энергии расщепился на три: невырожденный, один двукратно и один трехкратно вырожденный уровни энергии. Учет более высоких порядков теории возмущений уже не сможет качественно изменить картину.

Б-2.8.6 Скрещивание уровней

Уровни энергии невозмущенной системы зависят от параметра λ, и при некотором значении λ_0 два уровня энергии совпадают: $E_1^{(0)}(\lambda_0) = E_2^{(0)}(\lambda_0)$. В начальный момент времени система находится на первом уровне в состоянии $\psi_1^{(0)}$. Найти вероятность того, что система будет находиться в момент времени t в состоянии $\psi_2^{(0)}$, если на нее накладывается малое постоянное возмущение $\hat{\mathrm{V}}$. Считать, что матричные элементы $V_{11} = V_{22} = 0$, но $V_{12} = V_{21}^* \neq 0$.

Solution.

2.8.6. В невозмущенной задаче уровни энергии очень близки или совпадают, поэтому применим теорию возмущений для близких уровней энергии. Сформируем линейные комбинации волновых функций нулевого приближения $\tilde{\psi} = C_1\psi_1^{(0)} + C_2\psi_2^{(0)}$ и подставим их в уравнение $\left(\hat{\mathrm{H}}^{(0)} + \hat{\mathrm{V}}\right)\tilde{\psi} = E\tilde{\psi}$. В результате для нахождения коэффициентов C_1, C_2 мы получим систему

$$\begin{pmatrix} H_{11} - E & H_{12} \\ H_{21} & H_{22} - E \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0,$$

где введены обозначения

$$H_{mn} = \langle\psi_m^{(0)}|\hat{\mathrm{H}}|\psi_n^{(0)}\rangle = \begin{cases} V_{nn} + E_n^{(0)}, & m = n, \\ V_{mn}, & m \neq n. \end{cases} \quad m, n = 1, 2.$$

Вообще говоря, здесь не предлолагается, что уровни энергии в невозмущенной задаче совпадают, т. е. $E_1^{(0)} \neq E_2^{(0)}$. Из условия разрешимости системы (1) находим значения уровней энергии для линейных комбинаций $\widetilde{\psi}_{1,2}$:

$$E_{1,2} = \frac{1}{2}\left\{(H_{11} + H_{22}) \pm \hbar\omega\right\}, \quad \hbar\omega = \sqrt{(H_{11} - H_{22})^2 + 4|H_{12}|^2}.$$

Из системы (1) находим коэффициенты C_1, C_2, позволяющие построить функции $\widetilde{\psi}_{1,2} = C_1^{1.2}\psi_1^{(0)} + C_2^{1.2}\psi_2^{(0)}$, нормированные на единицу, т. е. Далее выразим $\psi_{1,2}^{(0)}$ через $\widetilde{\psi}_{1,2}$: $\psi_{1,2}^{(0)} = \mp\left(C_{2,1}^2\widetilde{\psi}_1 - C_{2,1}^1\widetilde{\psi}_2\right)$. Здесь мы учли, что $\det C = -1$. Функции $\widetilde{\psi}_{1,2}$ описывают состояния с определенной энергией, поэтому, восстанавливая зависимость от времени, получим

$$\Psi_1^{(0)}(x,t) = C_2^1\tilde{\psi}_2 e^{-\frac{i}{\hbar}E_2 t} - C_2^2\tilde{\psi}_1 e^{-\frac{i}{\hbar}E_1 t}.$$

Полученная нами волновая функция описывает состояние, в котором $\Psi_1^{(0)}(x,0) = \psi_1^{(0)}$, как и требуется по условию задачи. Подставим в соотношение (3) функции $\widetilde{\psi}_1$ и $\widetilde{\psi}_2$, выраженные через $\psi_{1,2}^{(0)}$. В результате получим функцию $\Psi_1^{(0)}(x,t)$ в виде разложения по состояниям $\psi_{1,2}^{(0)}$, причем коэффициенты разложения теперь будут зависеть от времени. В соответствии с вероятностной интерпретацией квадрат модуля коэффициента перед $\psi_2^{(0)}$ должен быть равен вероятности обнаружить систему в момент t в состоянии $\psi_2^{(0)}$:

$$W = |C_2^1 C_2^2\left[e^{-\frac{i}{\hbar}E_2 t} - e^{-\frac{i}{\hbar}E_1 t}\right]|^2 = \frac{2|H_{12}|^2}{(\hbar\omega)^2}[1 - \cos\omega t] = \frac{4\left[H_{12}\right|^2}{(\hbar\omega)^2}\sin^2\left(\frac{\omega t}{2}\right).$$

Здесь мы использовали соотношения (2).

Б-2.8.7 Переходы при β-распаде трития

Найти вероятность того, что при β-распаде трития ион $^3\mathrm{He}^+$ окажется: **а)** в 1s-состоянии; **б)** в 2s-состоянии; **в)** в 2p-состоянии, если атом трития находился в 1s-состоянии.

Solution.

(??? суть???)
β-Распад трития

$$^3_1\mathrm{H} \to {}^3_2\mathrm{He} + \mathrm{e}^- + \widetilde{\nu}_\mathrm{e}$$

представляет собой быстрый процесс, в течение которого изменяется потенциальная энергия электрона в атоме:

$$U_\mathrm{H}(r) = -\frac{e^2}{r} \quad \to \quad U_\mathrm{He}(r) = -\frac{2e^2}{r},$$

поскольку ядро трития превращается в ядро изотопа ^{3}He. Время распада можно оценить, как время пролета β-электрона через область, занимаемую атомом $t_\beta \sim a/v_\beta$, где a - радиус боровской орбиты, v_β – скорость β-электрона. Поскольку энергия β-электрона имеет порядок нескольких кэВ, то $v_\beta/c \sim 10^{-1} \gg v_\mathrm{at}/c \sim \alpha \simeq 1/137$, где $v_\mathrm{at} \sim e^2/\hbar$ - скорость атомных электронов. В итоге получаем, что t_β гораздо меньше характерных атомных времен:

$$t_\beta \sim \frac{a}{v_\beta} \sim \frac{\hbar^2}{me^2}\frac{1}{v_\beta} \ll \frac{\hbar^2}{me^2}\frac{1}{v_\mathrm{at}} \sim \frac{\hbar^3}{me^4} \sim \tau_\mathrm{aT}.$$

Это означает, что волновая функция электрона не успевает измениться за время t_β, в течение которого меняется потенциальная гамильтониана этой системы. Вместе с гамильтонианом меняется и система его собственных функций, поэтому мы можем разложить исходную волновую функцию электрона ψ^H в поле $U_\mathrm{H}(r)$ по собственным функциям в поле $U_\mathrm{He}(r)$:

$$\psi^\mathrm{H} = \sum_n C_n \psi_n^\mathrm{He} + \int C_\mathbf{k} \psi_\mathbf{k}^\mathrm{He} d\mathbf{k},$$

где коэффициенты разложения $C_n = \langle \psi_n^\mathrm{He} | \psi^\mathrm{H} \rangle = \int \psi_n^{\mathrm{He}*}\, \psi^\mathrm{H} d^3x$ определяют вероятности перехода электрона $w_n = |C_n|^2$ в одно из связанных состояний иона He.

Имея в виду явный вид радиальных функций электрона

$$R_{10} = 2\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-Zr/a_0}, \qquad R_{21} = \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_0}\right)^{\frac{3}{2}}\left(\frac{Zr}{a_0}\right) e^{-Zr/2a_0}$$

$$R_{20} = 2\left(\frac{Z}{2a_0}\right)^{\frac{3}{2}}\left(1 - \frac{Zr}{2a_0}\right) e^{-Zr/2a_0}, \qquad R_{32} = \frac{2\sqrt{2}}{27\sqrt{5}}\left(\frac{Z}{3a_0}\right)^{\frac{3}{2}}\left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$$

в тритии и в гелии имеем

$$R_{10}^\mathrm{H}(r) = \frac{2}{a^{3/2}} e^{-\frac{r}{a}}, \qquad R_{10}^\mathrm{He}(r) = \frac{4\sqrt{2}}{a^{3/2}} e^{-\frac{2r}{a}},$$

$$R_{20}^\mathrm{He}(r) = \frac{2}{a^{3/2}}\left(1 - \frac{r}{a}\right) e^{-\frac{r}{a}}, \quad R_{21}^\mathrm{He}(r) = \frac{2}{a^{3/2}}\frac{r}{a\sqrt{3}} e^{-\frac{r}{a}},$$

получим окончательно

$$w_{1s} = \left(\frac{16\sqrt{2}}{27}\right)^2 \simeq 0,70; \quad w_{2s} = \frac{1}{4}; \quad w_{2p} = 0.$$

Б-2.8.8 Эффект Мессбауэра через теорию возмущений (??)

Определить вероятность процесса, при котором ядро, связанное гармоническим потенциалом, останется в основном состоянии после испускания γ-кванта (эффект Мессбауэра).

Solution.

(??? суть???)
(!!! в теории укажу про этот эффект и про его применения!!! пока что про него почти ничего не написано там, это плохо.)
(??? решал кстати, давно не повторял это.)
При резонансном испускания γ-кванта ядром, переходящим из возбужденного состояния в основное, энергия испущенного γ-кванта ε_γ должна быть в точности равна энергии возбуждения ядра: $\varepsilon_\gamma = \varepsilon$. Известно, что для свободно движущегося ядра такой процесс не идет, потому что этому мешает отдача ядра, возникающая вследствие действия закона сохранения импульса (см. задачу 1.3.36). Оказалось, что в твердом теле связанные ядра-излучатели могут излучать γ-кванты «без отдачи». Причем процесс возможен именно потому, что ядро связано, а не свободно.
В дальнейшем рассмотрим простую одномерную модель, предполагающую, что ядро-излучатель связано гармоническим потенциалом:

$$\hat{\mathrm{H}} = \frac{\hat{\mathrm{p}}^2}{2M} + \frac{M\omega^2\hat{x}^2}{2}; \quad \hat{\mathrm{H}}|n\rangle = E_n|n\rangle, \quad E_n = \hbar\omega\left(n + \frac{1}{2}\right).$$

где M - масса ядра. Вектор $|n\rangle$ теперь характеризует состояние ядра в пространстве в целом.
В отличие от этого, если бы ядро было свободным, то его пространственное состояние следовало бы характеризовать собственным вектором оператора импульса $|k'\rangle$, где $\hat{p}|k'\rangle = \hbar k'|k'\rangle$. При испускании γ-кванта свободным ядром это состояние переходит в $|k' - k\rangle$, где $\hbar k$ - импульс испущенного γ-кванта.
При движении в гармоническом потенциале импульс уже не будет интегралом движения, и начальное состояние ядра $|n\rangle$ не является собственным вектором оператора импульса. Поэтому теперь невозможно применить закон сохранения импульса по схеме $|k'\rangle \to |k' - k\rangle$, как для свободного случая. Однако состояние ядра $|n\rangle$ можно разложить по собственным векторам оператора импульса:

$$|n\rangle = \int |k'\rangle\langle k'|n\rangle dk'.$$

Дальнейшие рассуждения будут существенным образом использовать тот факт, что рассматриваемый нами процесс является быстрым по сравнению с характерным временем движения в гармоническом потенциале. Приведем оценку времени взаимодействия. Длина волны γ-кванта намного больше размеров ядра, ибо $\hbar\omega_\gamma \sim \hbar c/\lambda_\gamma \ll \hbar c/R_{\text{ядра}} \simeq 40$ МэВ. Поэтому время взаимодействия можно оценить, как $\tau_\gamma \sim \lambda_\gamma/c \sim \omega_\gamma^{-1}$. Поскольку энергия γ-кванта гораздо больше характерной энергии колебаний ядра $\hbar\omega$ (см. (1)), то время взаимодействия τ_γ оказывается много меньше $\tau_{\text{ядра}} \sim \omega^{-1}$ - характерного времени эволюции состояния ядра в гармоническом потенциале.
На основании этого делаем вывод о том, что процесс испускания γ-кванта действительно является быстрым. Одновременно и так же быстро срабатывает и закон сохранения импульса. Поэтому можно считать, что в выражении (2) каждое состояние с определенным значением импульса $|k'\rangle$ получает сдвиг: $|k'\rangle \to |k' - k\rangle$. Коэффициенты в разложении не изменяются. Следовательно, вектор конечного состояния ядра можно записать в виде

$$|f\rangle = \int |k' - k\rangle\langle k'|n\rangle dk' = \int e^{-ik\hat{x}}|k'\rangle\langle k'|n\rangle dk' = e^{-ik\hat{x}}|n\rangle.$$

Очевидно, что состояние $|f\rangle$ не является собственным вектором гамильтониана (1), но его можно разложить по полной системе собственных векторов $\{|n\rangle\}$:

$$|f\rangle = e^{-ik\hat{x}}|n\rangle = \sum_{n'} |n'\rangle\langle n'|e^{-ik\hat{x}}|n\rangle.$$

Отсюда видно, что вероятность того, что ядро при испускании перейдет в одно из состояний гармонического осциллятора, равна

$$W_{n\to n'} = |\langle n'|e^{-ik\hat{x}}|n\rangle|^2.$$

Энергия испущенного γ-кванта при этом $\varepsilon_\gamma = \varepsilon - \hbar\omega\,(n' - n)$, где последнее слагаемое - это энергия, забираемая ядром. Случай $n' = n$ отвечает условию $\varepsilon_\gamma = \varepsilon$, следовательно, это и есть условие резонансного испускания. Вычислим вероятность резонансного испускания из основного состояния осциллятора:

$$W_{0\to 0} = |\langle 0|e^{-ik\hat{x}}|0\rangle|^2 = \left|\frac{1}{x_0\sqrt{\pi}}\int\limits_{-\infty}^{+\infty} e^{-ikx}e^{-\left(\frac{x}{x_0}\right)^2}dx\right|^2 = e^{-\frac{x_0^2k^2}{2}}.$$

Мы получили так называемый фактор Дебая-Уоллера.

Куда девается энергия при эффекте Мессбауэра (??)

(!!! в теорию отнесу потом этот вопрос, тут тупо задача на метод.)

ПТФ-5.пр.1.2 Сжатие сферы с бесконечными стенками (?)

(!!! укажу и во введении и в других местах, почему именно так такую задачу решают!! потом напишу ее!!)

(первый порядок теории возмущений)

Пусть $U(\boldsymbol{r}) = \begin{cases} 0, & |\boldsymbol{r}| < R \\ \infty, & |\boldsymbol{r}| > R \end{cases}$

Гамильтониан можно записать через недеформированный как:

$$\hat{H} = \frac{\hat{p}^2}{2m} = \frac{\hat{p}^2}{2m} + \frac{\hat{p}_z^2}{2m}\left(\left(\frac{r}{R'}\right)^2 - 1\right) \approx \underbrace{\frac{\hat{p}^2}{m}}_{\hat{H}_0} + \underbrace{\frac{\hat{p}_z^2 \epsilon}{m}}_{\hat{V}}$$

Уравнение Шредингера:

$$-\frac{1}{2m}\left(\frac{\partial^2\psi}{\partial r^2} + \frac{2}{r}\frac{\partial\psi}{\partial r}\right) = E\psi(r), \quad \psi(r=R) = 0$$

(?? дальше не улавливаю суть)

$$-\frac{1}{2m}\chi''(r) = E\chi(r) \to \chi(r) = A\sin(kr) + B\cos(kr), \quad \frac{k^2}{2m} = E$$

$$\int_0^r 4\pi r^2 dr \cdot \frac{\sin^2 kr}{r^2} = 2\pi R \to \psi(r) = \frac{1}{\sqrt{2\pi r}}\frac{\sin kr}{r}$$

$$E_0^{(1)} = \frac{\pi^2}{3mR^3}\epsilon$$

Указания на общий метод решения задач с сжатием размеров (???)

(по идее это в теории напишу)

Г-8.15. Стационарные состояния в Кулоне с а) $U_0/\left(e^{r/a}-1\right)$, б) $-U_0 a e^{-r/a}/r$

Частица находится в центральном потенциале вида а) $U = -U_0/\left(e^{r/a}-1\right)$ б) $U = -U_0 a e^{-r/a}/r$, причем $U_0 \gg \hbar^2/ma^2$. В первом порядке теории возмущений найти отличие энергетических уровней нижней части спектра от уровней в кулоновском поле $U = -U_0 a/r$. Обратить внимание на снятие случайного кулоновского вырождения уровней.

Solution.

8.15. При $r \ll a$ рассматриваемые потенциалы имеют вид $U \approx -U_0 a/r$. В таком кулоновском поле в. ф. нижних энергетических уровней локализованы на расстоянии порядка $r_n \sim a_0 n^2$ от центра поля; здесь $a_0 = \hbar^2/m^2 U_0, n$ - главное квантовое число. Если $r_n \ll a$ (т. е. $\xi \equiv ma^2U_0/\hbar^2 \gg n^2$), то, очевидно, в нулевом приближении искомые уровни нижней части спектра и соответствующие им с.ф. будут такие же, как и в кулоновском поле:

$$E_{n_r l}^{(0)} = -\frac{ma^2U_0^2}{2\hbar^2 n^2}, \quad \Psi_{n_r lm}^{(0)} = \Psi_{n_r lm}^{\text{Ky}J},$$

см. (IV.3). При этом отличие рассматриваемых потенциалов от кулоновского играет роль возмущения $V(r) = U(r) + U_0 a/r$. Ввиду того что орбитальный момент частицы является интегралом движения и при действии возмущения, с.ф. (1) являются правильными функциями нулевого прибінжения и поправка первого порядка определяется выражением

$$E_{n_r l}^{(1)} = \int V(r)|\Psi_{n_r lm}^{(0)}|^2 d^3r.$$

а) Разлагая потенциал возмущения в ряд по степеням r/a, что дает и учитывая значение интеграла (см. [1, §36]) согласно (2) - (4) находим

$$E_{n_r l}^{(1)} = U_0\left\{\frac{1}{2} - \frac{3n^2 - l(l+1)}{24\xi}\right\}, \quad n = n_r + l + 1$$

6) Теперь $V \approx U_0\left(1 - r/2a + r^2/6a^2\right)$ и

$$E^{(1)}_{n_r l} = U_0\left\{1 - \frac{3n^2 - l(l+1)}{4\xi} + \frac{n^2}{12\xi^2}\left[5n^2 + 1 - 3l(l+1)\right]\right\}.$$

Как видно из (5) и (6), случайное кулоновское вырождение уровней по l снимается.

Заметим, что для потенциала Хюльтена у. Ш. для s-состояний допускает точное решение, см. 4.8. При этом (для $l = 0$) $E^{(0)}_{n_r 0}$ совместно с (5) описывают точный результат.

ADD PROBLEMS FROM GALITSKI!!!

17.1.3 Problems about Time-Independent PT 3

Г-8.16.

Для частицы в центральном потенциале $U = -\alpha/r^v$, причем $0 < v < 2$, найти энергетические уровни $E_{n_r l}$ с большим значением момента $l \gg 1$ и с не слишком большим радиальным квантовым числом n_r. В случае кулоновского потенциала, $v = 1$, сравнить полученный результат с точным.

Solution.

Г-8.17.

То же, что и в предыдущей задаче, но для потенциала $U = \alpha r^v$ с $\alpha, v > 0$ (теперь $E_{n_r l} > 0$). В случае сферического осциллятора, $v = 2$, сравнить полученный результат с точным.

Solution.

Г-8.18.

Частица находится внутри непроницаемого эллипсоида вращения, так что потенциал имеет вид

$$U(x,y,z) = \begin{cases} 0, & \left(x^2+y^2\right)/a^2 + z^2/b^2 < 1, \\ \infty, & \left(x^2+y^2\right)/a^2 + z^2/b^2 \geqslant 1, \end{cases}$$

причем $|a - b| \ll a$. Найти в первом порядке теории возмущений сдвиг основного энергетического уровня по отношению к уровню в сферической яме такого же объема.

Solution.

Г-8.19.

Обобщить результат предыдущей задачи на случай возбужденных состояний частицы. Обсудить вопрос о характере снятия вырождения по проекциям момента в первом и более высоких порядках теории возмущений.

Solution.

Киселев-?(m) Два уровня, один из которых вырожден

Рассмотрим систему, гамильтонан которой представляет собой матрицу 3×3, которая описывает двукратно вырожденный уровень энергии E_1 и отделённый от него энергетической щелью уровень энергии E_2. Недиагональные элементы гамильтониана - возмущение, дающее туннелирование между этими уровнями энергии, и оно не снимает вырождение в первом порядке теории возмущений:

$$\hat{H} = \begin{pmatrix} E_1 & 0 & t_1 \\ 0 & E_1 & t_2 \\ t_1 & t_2 & E_2 \end{pmatrix}, \quad |\Delta| = |E_2 - E_1| \gg t^2_{1,2}$$

Определить уровни энергии.

Solution.

Разумеется, задачу эту можно решить точно. Точные собственные значения записываются следующим образом:

$$E = \left\{ E_1, \quad \frac{1}{2}\left(E_1 + E_2\right) \pm \sqrt{(\Delta/2)^2 + |t_1|^2 + |t_2|^2} \right\} \approx \left\{ E_1 - \frac{t_1^2 + t_2^2}{\Delta}, \quad E_1, \quad E_2 + \frac{t_1^2 + t_2^2}{\Delta} \right\}$$

Поскольку возмущение не связывает состояния с вырожденного подпространства, то можно было бы попробовать наивно применить второй порядок невырожденной теории возмущений (5.8):

$$E_{1,1}^{(2)} = \frac{|V_{13}|^2}{E_1 - E_2} = -\frac{t_1^2}{\Delta}, \quad E_{1,2}^{(2)} = \frac{|V_{23}|^2}{E_1 - E_2} = -\frac{t_2^2}{\Delta}, \quad E_2^{(2)} = \frac{|V_{31}|^2}{E_2 - E_1} + \frac{|V_{32}|^2}{E_2 - E_1} = \frac{t_1^2 + t_2^2}{\Delta}$$

что для уровня энергии E_2 даёт правильный ответ, а для вырожденного уровня E_1 - нет. Чтобы получить правильные ответы, необходимо пользоваться вторым порядком вырожденной теории возмущений. Рецепт говорит, что необходимо составить эффективный гамильтониан для первых двух уровней:

$$H_{11}^{(\text{eff})} = \frac{V_{13}V_{31}}{E_2 - E_1} = -\frac{t_1^2}{\Delta}, \quad H_{12}^{(\text{eff})} = H_{21}^{(\text{eff})} = \frac{V_{13}V_{32}}{E_2 - E_1} = -\frac{t_1 t_2}{\Delta}, \quad H_{22}^{(\text{eff})} = \frac{V_{23}V_{32}}{E_2 - E_1} = -\frac{t_2^2}{\Delta} =$$

поэтому

$$\hat{H}^{(\text{eff})} = -\frac{1}{\Delta}\begin{pmatrix} t_1^2 & t_1 t_2 \\ t_1 t_2 & t_2^2 \end{pmatrix}$$

Диагонализуя матрицу, мы получаем поправки второго порядка к вырожденному уровню:

$$E_{1,1}^{(2)} = 0, \quad E_{1,2}^{(2)} = -\frac{t_1^2 + t_2^2}{\Delta}$$

которые на сей раз воспроизводят правильный ответ (5.27), полученный из точного решения. Наивный же подход не учитывает недигональные элементы матрицы эффективного гамильтониана, которые дают вклад того же порядка, что и диагональные.

Landau-Inst-summer-2025.8/8. Repulsive ball in a sphere

A particle of mass m is in the ground state in a spherical cavity of radius R with infinite walls:

$$U(\boldsymbol{r}) = \begin{cases} 0, & r < R, \\ \infty, & r \geqslant R. \end{cases}$$

To an arbitrary point $\boldsymbol{r}_0$ inside the sphere, located at a distance of $r_0 < (R - a)$ from the center, an impurity is placed, which is an impenetrable ball of radius $a \ll R$:

$$\delta U(\boldsymbol{r}) = \begin{cases} 0, & |\boldsymbol{r} - \boldsymbol{r}_0| > a, \\ \infty, & |\boldsymbol{r} - \boldsymbol{r}_0| \leqslant a. \end{cases}$$

Determine the energy shift of the ground state in the first non-vanishing order by a.

Solution.

(??? a really good problem, I'll think when I work out theory and other problems)
I guess one needs to use first order perturbation theory and evaluate accurately the integral, by approximating it by delta-function with strength that is depended a.
(???)

17.1.4 Problems about Time-Dependent PT 1

ADD PROBLEMS FROM GALITSKI!!!

Leuven-s6.ex1 The two-state system

Consider a two-state system with the Hamiltonian $H_0 = \begin{pmatrix} E_1^0 & 0 \\ 0 & E_2^0 \end{pmatrix}$ with a time-dependent perturbation $V = \begin{pmatrix} 0 & \lambda\cos(\omega t) \\ \lambda\cos(\omega t) & 0 \end{pmatrix}$, with $\lambda \in \mathbb{R}$ and little.

At $t = 0$ the system is known to be in the first state $|1\rangle$ represented by $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

Assume that $E_1^0 - E_2^0$ is not close to $\pm\hbar\omega$, derive an approximate expression for the probability that the system is found in the state $|2\rangle$ as a function of time ($t > 0$).

Why is this procedure not valid when $E_1^0 - E_2^0$ is close to $\pm\hbar\omega$?

Solution

We use the framework of time-dependent perturbation theory, and we already have formulas for the change of the wavefunction, thus we just plug there our perturbation and get the answer.

1. We need $|c_2^{(1)}(t)|^2$, where

$$c_2^{(1)}(t) = -\frac{i}{\hbar}\int_0^t e^{i\omega_{21}t'}\langle 2|\hat{V}|1\rangle dt' = -\frac{i}{\hbar}\int_0^t e^{i\omega_{21}t'}\lambda\cos(\omega t')\,dt' = \frac{i\lambda}{2\hbar}\int_0^t e^{i(\omega_{21}-\omega)t'} + e^{i(\omega_{21}+\omega)t'}\,dt'$$

We introduce $\omega_\pm = \omega_{21} \pm \omega$, so the coefficient is given by

$$c_2^{(1)} = -\frac{\lambda}{2\hbar}\left[\frac{e^{i\omega_- t} - 1}{\omega_-} + \frac{e^{i\omega_+ t} - 1}{\omega+}\right]$$

After some algebra (write it!!), we have

$$|c_2^{(1)}|^2 = \frac{\lambda^2}{\hbar^2}\left[\frac{\sin^2(\omega_- t/2)}{\omega_-^2} + \frac{\sin^2(\omega_+ t/2)}{\omega_+^2} + \frac{\cos(\omega t)\left(\cos(\omega t) - \cos(\omega_{21} t)\right)}{\omega_{21}^2 - \omega^2}\right]$$

2. If $E_1^0 - E_2^0$ is close to $\pm\hbar\omega$, then $\omega_{21}^2 - \omega^2 \approx 0$, so the perturbative framework is no longer valid.
(???? what it the limit of littleness of λ???)

Г-8.33.

Заряженный линейный осциллятор подвергается воздействию однородного электрического поля, изменяющегося во времени по закону: а) $\mathscr{E}(t) = \mathscr{E}_0\exp\left(-t^2/\tau^2\right)$, б) $\mathscr{E}(t) = \mathscr{E}_0\left(1 + t^2/\tau^2\right)^{-1}$, в) $\mathscr{E}(t) = \mathscr{E}_0\exp\left(-t^2/\tau^2\right)\cos\omega_0 t$. Считая, что до включения поля (при $t \to -\infty$) осциллятор находился в n-м квантовом состоянии, найти в первом порядке теории возмущений вероятности возбуждения различных его состояний при $t \to +\infty$. Для случая $n = 0$ сравнить полученный результат с точным, см. 6.25.

Solution.

(add the original solution and problem in English!)

Г-8.34.

На плоский ротатор, имеющий дипольный момент d, накладывается однородное, переменное во времени электрическое поле $\mathscr{E}(t) = \mathscr{E}(t)\mathbf{n}_0$. До включения поля ротатор имел определенное значение энергии и проекции момента m. Вычислить в первом порядке теории возмущений вероятности различных значений проекции момента и энергии ротатора при $t \to +\infty$. Рассмотреть конкретные виды $\mathscr{E}(t)$, указанные в предыдущей задаче.

Solution.

(add the original solution and problem in English!)

Г-8.35.

То же, что и в предыдущей задаче, но для сферического ротатора. До включения электрического поля ротатор находился в состоянии с квантовыми числами $l, l_z = m$; поле направлено вдоль оси z.

Solution.

(add the original solution and problem in English!)

Г-8.36.

В условиях задачи 8.34 рассмотреть переходы ротатора в случае, когда вектор электрического поля вращается в плоскости вращения ротатора с угловой скоростью ω_0, так что $\mathscr{E}_x = \mathscr{E}(t)\cos\omega_0 t, \mathscr{E}_y = \mathscr{E}(t)\sin\omega_0 t$. Обратить внимание на возможность существенного возрастания вероятности перехода даже в случае «Плавной» зависимости $\mathscr{E}(t)$ вида) и б) из 8.33.

Solution.

(add the original solution and problem in English!)

Г-8.37.

Получить выражения для волновой функции и амплитуды перехода системы из начального. (при $t \to -\infty$) n-го состояния дискретного спектра в ко-

Solution.

(add the original solution and problem in English!)

Б-2.8.9 δ-potential with $\hat{\mathrm{V}}(t) = Fx\cos\omega t$

Find the probability of transition of a particle in a bound state in the field of a δ well into a continuous spectrum under the influence of an external field of the form $\hat{\mathrm{V}}(t) = Fx\cos\omega t$ in the case when $\hbar\omega > \hbar^2\varkappa_0^2/(2m)$.

Solution.

We use Fermi golden rule (since we have a periodic potential), for which we just compute the matrix element and known properties of delta-potential.

$$\hat{\mathrm{H}} = \frac{\hat{\mathrm{p}}^2}{2m} - \frac{\hbar^2}{m}\varkappa_0\delta(x) + \frac{Fx}{2}\left(e^{i\omega t} + e^{-i\omega t}\right).$$

$$\psi_0^{(0)}(x) = \sqrt{\varkappa_0}e^{-\varkappa_0|x|}, \qquad E_0^{(0)} = E_0 = -\frac{\hbar^2\varkappa_0^2}{2m}$$

$$w = \frac{2\pi}{\hbar}\int |F_{\nu 0}|^2\delta\left(E_\nu - E_0 - \hbar\omega\right)d\nu,$$

где ν - квантовое число, нумерующие состояния непрерывного спектра. Прежде всего рассмотрим случай $\hbar\omega \gg |E_0|$, т. е. приближение, когда δ-потенциал не действует на частицу в конечном состоянии. Тогда в качестве волновой функции конечного состояния можно просто выбрать функцию свободной частицы:

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}}e^{ikx}, \qquad \nu = k \in (-\infty, \infty), \qquad E_k = \frac{\hbar^2k^2}{2m}.$$

$$F_{k0} := \langle\psi_0^{(0)}|\frac{Fx}{2}|\psi_k(x)\rangle = \frac{F\sqrt{\varkappa_0}}{2\sqrt{2\pi}}\int\limits_{-\infty}^{\infty} xe^{-\varkappa_0|x|+ikx}dx = i\frac{2F\varkappa_0^{3/2}k}{\sqrt{2\pi}\left(k^2+\varkappa_0^2\right)^2},$$

(we take away the time-dependent part of the perturbation (?? why??))

After using $\delta(f(x)) = \sum_{i=1}^{n} \frac{\delta(x-x_i)}{|f'(x_i)|}$, one gets (??? do it!!)

$$w = \frac{2\pi}{\hbar}\left[|F_{k_10}|^2 + |F_{k_20}|^2\right]\left|\frac{dE_k}{dk}\right|^{-1}, \qquad k_{1,2} = \pm\frac{1}{\hbar}\sqrt{2m\left(\hbar\omega + E_0\right)}.$$

(do computations here!)

$$w = \frac{2\hbar F^2}{m(\hbar\omega)^4}|E_0|^{3/2}\sqrt{\hbar\omega - |E_0|}.$$

Solution for the case $\hbar\omega \gtrsim |E_0|$

In this case, it is necessary to choose the exact eigenfunctions of the undisturbed Hamiltonian (for a continuous spectrum) as the zero approximation functions. Since the undisturbed Hamiltonian commutes with the inversion operator, even and odd functions can be considered separately. Obviously, even functions will give zero contribution to the matrix element. Odd solutions have the form $\psi_k(x) = (1/\sqrt{\pi})\sin kx$. Calculating the probability with these functions leads us back to the formula

$$w = \frac{2\hbar F^2}{m(\hbar\omega)^4}|E_0|^{3/2}\sqrt{\hbar\omega - |E_0|}.$$

(??? do the computations)

And if there $\hbar\omega < |E_0|$, there will be never a transfer to continuum state.

Б-2.8.10 Transition in $V(t) = \frac{V_0}{2}\left(1 + \frac{2}{\pi}\operatorname{arctg}\frac{t}{\tau}\right)$

Find the formula for a probability of transition between states of a discrete spectrum of an abstract quantum system under $V(t) = \frac{V_0}{2}\left(1 + \frac{2}{\pi}\operatorname{arctg}\frac{t}{\tau}\right)$.

Solution.

We use the basic time-dependent perturbation theory.

$$W_{fi}(t) = \frac{1}{\hbar^2}\left|\int\limits_{-\infty}^{t} V_{fi}\left(t'\right)e^{i\omega_h t'}dt'\right|^2 \equiv \frac{|V_{0ji}|^2}{4\hbar^2}|I(t)|^2,$$

(??? what is I?)

Here, the upper limit of the integral t must be further limited to infinity. In order not to get a divergence, we integrate by parts

$$I(t) = \frac{e^{i\omega_{fi}t'}}{i\omega_{fi}}\left[1 + \frac{2}{\pi}\operatorname{arctg}\frac{t'}{\tau}\right]\Bigg|_{-\infty}^{t} - \frac{2\tau}{i\pi\omega_{fi}}\int\limits_{-\infty}^{t}\frac{e^{i\omega_{fi}t'}dt'}{t'^2+\tau^2}.$$

Here, the first term describes the correction of the first approximation to the initial wave function at $t > 0$ and does not contribute to the transitions. (??? why?? this is how we get rid of infinities!)

Quantum transitions are described by the second term, and after striving $t \to \infty$, the integral is taken by (???? I forgot, how to take it???? write here! by residues https://www.youtube.com/watch?v=jpT0maiGZAY&ab_channel=CrystalMath...) Anyway, we use $\int_{-\infty}^{\infty}\frac{e^{itx}}{1+x^2}dx = \begin{cases}\pi e^{-t}, & \text{for } t > 0\\ \pi, & \text{for } t = 0\end{cases}$ and we get

$$W'_{fi} = \frac{|V_{0fi}|^2}{\hbar^2\omega_{fi}^2}e^{-2\omega_{fi}\tau}.$$

Б-2.8.11 Oscillator and increasing field

For a charged linear harmonic oscillator that is initially in the ground state, determine the probabilities of transitions to various excited states under the influence of a homogeneous electric field of the form

$$\mathcal{E} = \begin{cases}0, & t < 0,\\ \mathcal{E}_0\frac{t}{\tau}, & 0 \leqslant t \leqslant \tau,\\ \mathcal{E}_0, & t > \tau\end{cases}$$

Consider the limits of instantaneous and slow field activation.

Solution.

This problem is typical for time-dependent perturbation theory, one needs to apply basic formulas and also get rid of some typical divergence of an integral.

$$\hat{\mathrm{H}} = \frac{\hat{\mathrm{p}}^2}{2m} + \frac{m\omega^2 x^2}{2} - e\mathcal{E}x,$$

$$a_{0n}^{(1)} = \frac{1}{i\hbar}\int\limits_{-\infty}^{t} V_{n0}\left(t'\right) e^{i\omega_{n0}t'}dt' \overset{\text{i b p}}{=} i\int\limits_{-\infty}^{t} \frac{\partial V_{n0}\left(t'\right)}{\partial t'}\frac{e^{i\omega_{n0}t'}}{\hbar\omega_{n0}}dt' + \text{const.}$$

Here we said that the first term after i.b.p. is zero (??? think more, why exactly it is so???)

The only nonzero matrix element is

$$V_{10} = -e\mathcal{E}\langle 1|\hat{x}|0\rangle = -\frac{e\mathcal{E}x_0}{\sqrt{2}}, \qquad x_0 := \sqrt{\frac{\hbar}{m\omega}}.$$

$$W_{0\to 1} = W_0\frac{\sin^2\left(\frac{\omega\tau}{2}\right)}{\left(\frac{\omega\tau}{2}\right)^2}, \qquad W_0 := \frac{e^2\varepsilon^2}{2\hbar m\omega^3}.$$

В случае мгновенного включения поля ($\omega\tau \ll 1$) имеем $W_{0\to 1} \simeq W_0$.

При адиабатически медленном включении поля ($\omega\tau \gg 1$) получим $W_{0\to 1} \simeq 0$, т. е. переходы в возбужденные состояния практически не происходят.

Б-2.8.12 Muon in a rotating field

Muon, which is at rest in a strong homogeneous magnetic field $\mathcal{H}_0 \| z$, is affected by a weak circularly polarized radio frequency field $\mathbf{h}(t) \perp \mathcal{H}_0$. Find the time dependence of the spin function $\chi(t)$ and the muon polarization $\mathbf{P}(t) = \langle\chi(t)|\hat{\sigma}|\chi(t)\rangle$, if at the initial moment $\chi(0) = \chi_{1/2}$.

Hint: here the muon is just a particle with spin 1/2, and only spin component of it is affected by a magnetic field. It has interaction with magnetic field by a magnetic dipole term.

Solution by perturbation theory

The model is as follows:

$$ih\frac{\partial}{\partial t}\chi(t) = \hat{\mathrm{H}}\chi(t),$$

and the interaction with the field is

$$\hat{\mathrm{H}} = -\mu_0(\hat{\boldsymbol{\sigma}}\boldsymbol{\mathcal{H}})\chi(t) = -\mu_0\left(\hat{\sigma}\mathcal{H}_0\right) - \mu_0(\hat{\boldsymbol{\sigma}}\mathbf{h}) = \underbrace{-\mu_0\left(\hat{\boldsymbol{\sigma}}\boldsymbol{\mathcal{H}}\right)}_{\hat{\mathrm{H}}_0}\underbrace{-\mu_0 h\left(\hat{\sigma}_x\cos\omega t + \hat{\sigma}_y\sin\omega t\right)}_{\hat{\mathrm{V}}(t)}. \quad \omega_0 := \gamma\mathcal{H}_0, \quad \gamma := e/(mc)$$

Here

$$\hat{\mathrm{H}}_0 = -\mu_0\mathcal{H}_0\hat{\sigma}_z = -\left(\hbar\omega_0/2\right)\hat{\sigma}_z,$$

and we used the gyromagnetic ratio $\mu_0 = \gamma\hbar/2$.

At the zero order one has

$$\hat{\mathrm{H}}_0\chi^{(0)} = E^{(0)}\chi^{(0)}; \quad E_{1,2}^{(0)} = \mp\mu_0\mathcal{H}_0 = \mp\frac{\hbar\omega_0}{2}, \quad \chi_{1,2}^{(0)} = \chi \pm 1/2.$$

(??? calculate the matrix element here!!!! just multiply matrices by raw and column, it should be very easy)
(check that $V_{11} = 0$, thus $a_{11} = 0$)

$$a_{12}^{(1)} = \frac{1}{i\hbar}\int\limits_0^t V_{21}\left(t'\right)e^{i\omega_0 t'}dt' \overset{\omega_1 := \gamma h}{=} -\frac{\omega_1}{2i}\int\limits_0^t e^{i(\omega+\omega_0)t'}dt' = \frac{\omega_1}{2\left(\omega+\omega_0\right)}\left(e^{i(\omega+\omega_0)t} - 1\right),$$

Thus

$$\chi(t) \approx \begin{pmatrix} e^{i\frac{\omega_0 t}{2}} \\ \frac{\omega_1}{2(\omega+\omega_0)}\left(e^{i(\omega+\omega_0)t} - 1\right)e^{-i\frac{\omega_0 t}{2}} \end{pmatrix}.$$

The conditions of applicability of perturbation theory is $|a_{12}^{(1)}|$ $ll1$. This can be implemented either with $\omega_1 \ll |\omega+\omega_0|$, i.e. the system must be far from resonance: $\omega \not\approx -\omega_0$, or with a short duration of the disturbance. Both options do not allow us to consider resonant phenomena in detail, thus one needs to have a better solution then perturbation theory.

Exact solution

The model is as follows:

$$ih\frac{\partial}{\partial t}\chi(t) = \hat{\mathrm{H}}\chi(t),$$

and the interaction with the field is

$$\hat{\mathrm{H}} = -\mu_0(\hat{\boldsymbol{\sigma}}\boldsymbol{\mathcal{H}})\chi(t) = -\mu_0\left(\hat{\sigma}\mathcal{H}_0\right) - \mu_0(\hat{\boldsymbol{\sigma}}\mathbf{h}) = \underbrace{-\mu_0\left(\hat{\boldsymbol{\sigma}}\boldsymbol{\mathcal{H}}\right)}_{\hat{\mathrm{H}}_0}\underbrace{-\mu_0 h\left(\hat{\sigma}_x\cos\omega t + \hat{\sigma}_y\sin\omega t\right)}_{\hat{\mathrm{V}}(t)}. \quad \omega_0 := \gamma\mathcal{H}_0, \quad \gamma := e/(mc)$$

Here

$$\hat{\mathrm{H}}_0 = -\mu_0\mathcal{H}_0\hat{\sigma}_z = -\left(\hbar\omega_0/2\right)\hat{\sigma}_z,$$

We solve as

$$\chi(t) := \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} \qquad \begin{cases} i\dot{C}_1 = -\dfrac{\omega_0}{2}C_1 - \dfrac{\omega_1}{2}e^{-i\omega t}C_2, \\ i\dot{C}_2 = -\dfrac{\omega_1}{2}e^{i\omega t}C_1 + \dfrac{\omega_0}{2}C_2, \end{cases} \qquad \begin{cases} C_1(0) = 1, \\ C_2(0) = 0, \end{cases}.$$

We substitute

$$C_1 = e^{-\frac{1}{2}\omega t}a, \qquad C_2 = e^{\frac{1}{2}\omega t}b$$

to get rid of time-dependence and get

$$\frac{d}{dt}\begin{pmatrix} a \\ b \end{pmatrix} = -i\begin{pmatrix} \varepsilon & \omega_1 \\ \omega_1 & -\varepsilon \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}, \qquad \begin{pmatrix} a(0) \\ b(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \varepsilon := \omega + \omega_0.$$

$$\begin{pmatrix} a \\ b \end{pmatrix} \equiv e^{i\Lambda t}\begin{pmatrix} 1 \\ 0 \end{pmatrix}; \qquad \Lambda := \begin{pmatrix} \varepsilon & \omega_1 \\ \omega_1 & -\varepsilon \end{pmatrix} \equiv \Omega\begin{pmatrix} \varepsilon/\Omega & \omega_1/\Omega \\ \omega_1/\Omega & -\varepsilon/\Omega \end{pmatrix}, \qquad \Omega := \sqrt{\varepsilon^2 + \omega_1^2}.$$

Because $\Lambda^2 = \Omega^2 \cdot \mathbf{1}$, all even powers of the matrix Λ will be proportional to the identity matrix, and we arrive at the relation (??? check!!)

$$e^{i\Lambda t} = \cos\Omega t\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + i\frac{\sin\Omega t}{\Omega}\begin{pmatrix} \varepsilon & \omega_1 \\ \omega_1 & -\varepsilon \end{pmatrix} = \cos\Omega t + i\frac{\Lambda}{\Omega}\sin\Omega t.$$

So, we have:

$$\begin{pmatrix} a \\ b \end{pmatrix} = \cos\Omega t\begin{pmatrix} 1 \\ 0 \end{pmatrix} + i\frac{\sin\Omega t}{\Omega}\begin{pmatrix} \varepsilon \\ \omega_1 \end{pmatrix}.$$

Thus, the answer is

$$\chi(t) = \begin{pmatrix} \left[\cos\left(\frac{\Omega}{2}t\right) + i\frac{\varepsilon}{\Omega}\sin\left(\frac{\Omega}{2}t\right)\right]e^{-i\frac{\omega}{2}t} \\ i\frac{\omega_i}{\Omega}\sin\left(\frac{\Omega}{2}t\right)e^{i\frac{\omega}{2}t} \end{pmatrix}.$$

Вероятность переворота спина, вычисленная при помощи данной функции, в точности совпадает с найденной в задаче 2.5.6. Реализация условия $\omega_1 \ll |\varepsilon|$ позволяет получить результат теории возмущений (3). Точный и приближенный результаты согласуются также и при малом времени действия возмущения $\Omega 2t \ll 1$.

Приведем также значения проекций вектора поляризации мюона:

$$\begin{aligned} \mathrm{P}_x &= \sin\theta[\cos\theta(1-\cos\Omega t)\cos\omega t - \sin\Omega t\sin\omega t], \\ \mathrm{P}_y &= \sin\theta[\cos\theta(1-\cos\Omega t)\sin\omega t + \sin\Omega t\cos\omega t], \\ P_z &= \cos^2\theta + \sin^2\theta\cos\Omega t \end{aligned}$$

где $\sin\theta = \omega_{\mathrm{I}}/\Omega, \cos\theta = \varepsilon/\Omega$, что совпадает с обозначениями задачи 2.5.6.

(?? it should be easy to derive it, do it!!)

Заметим, что фактически мы нашли оператор эволюции для данной задачи, который, как нетрудно сообразить, будет иметь вид $\hat{\mathrm{U}}(t) = e^{-\frac{t}{2}\omega\hat{\sigma}_z t}e^{i\Lambda t}$, где первая экспонента отвечает начальной замене переменных (переходу $C_1, C_2 \to a, b$). Подумайте, совпадает ли этот оператор с оператором эволюции, полученным другим методом в задаче 2.5.6.

Solution with circular motion

(??? the particle is also moving, right? Why one does not consider this??? or maybe it does not affect spin component anyway?)

ПТФ-8.з1. Осцилляция Раби

An alternating electric field is applied to the hydrogen atom in the ground state. $\hat{V} = -e\mathcal{E}\hat{z}\cos(\omega t)$, with the frequency near $\frac{3}{4}$Ry, which we write by introduction of a little frequency ε as $\omega = \frac{3}{4}\text{Ry} + \varepsilon$. The field satisfies $e\mathcal{E}a$, $\varepsilon \ll$ Ry. The ratio of the $\mathcal{E}$ field and the ε frequency tuning is, generally speaking, arbitrary. Determine the probability of detecting a particle in the ground and first excited states $n = 1$ and $n = 2$ after a long time T.

Reminder: Ry $= \frac{me^4}{2\hbar^2}$ – постоянная Ридберга, а $a = \frac{1}{me^2}$ – Боровский радиус.

Solution.

This problem is a typical for time-dependent PT.

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = (\hat{H}_0 + \hat{V}(t))|\psi(t)\rangle$$

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{r}, \quad \hat{V}(t) = -e\mathcal{E}\hat{z}\cos(\omega t), \quad \hat{z} = r\cos\theta$$

Эволюция основного и возбуждённого состояний, если бы не было возмущения: (??? check that indeed energies are indeed so)

$$|\psi_1(t)\rangle = e^{-\frac{\text{iRyt}}{\hbar}}|\psi_1\rangle, \quad |\psi_2(t)\rangle = e^{-\frac{\text{iRyt}}{4\hbar}}|\psi_2\rangle$$

Нестационарная теория возмущений:

$$i\hbar\frac{\partial\psi_2}{\partial t} = V_{21}\psi_1(t), \quad V_{21} = \langle\psi_2(t)|\hat{V}(t)|\psi_1(t)\rangle$$

$$i\hbar\frac{\partial\psi_2}{\partial t} = -e\mathcal{E}\cos(\omega t)e^{\frac{3i\text{Ryt}}{4\hbar}}\langle\psi_2|r\cos\theta|\psi_1\rangle\psi_1(t)$$

$$\langle\psi_2|r\cos\theta|\psi_1\rangle = \iint d\Omega r^3\cos\theta R_{2,1}Y_{1,0}R_{1,0}Y_{0,0} = \frac{2^6\sqrt{2}a}{3^4}$$

(?? check!!)

Остальные усреднения с ψ_2 при $n = 2$: $l = 0, m = 0$, $l = 1, m = -1$, $l = 1, m = 1$ дают 0 ввиду нечётности по углу θ. (??check!)

$$i\hbar\frac{\partial\psi_2}{\partial t} = -e\mathcal{E}(e^{i\omega t} + e^{-i\omega t})e^{\frac{3i\text{Ryt}}{4\hbar}}\frac{2^5\sqrt{2}a}{3^4}\psi_1(t) \approx 0 - e\mathcal{E}e^{-\frac{i\epsilon t}{\hbar}}\frac{2^5\sqrt{2}a}{3^4}\psi_1(t),$$

here we пренебрегли быстроосциллирующим слагаемым.

The same way one gets (check!!)

$$i\hbar\frac{\partial\psi_1}{\partial t} = -e\mathcal{E}e^{\frac{i\epsilon t}{\hbar}}\frac{2^5\sqrt{2}a}{3^4}\psi_2(t)$$

Totally, one has:

$$\frac{\partial\psi_1}{\partial t} = i\frac{e\mathcal{E}a}{\hbar}e^{\frac{i\epsilon t}{\hbar}}\frac{2^5\sqrt{2}}{3^4}\psi_2(t),$$
$$\frac{\partial\psi_2}{\partial t} = i\frac{e\mathcal{E}a}{\hbar}e^{-\frac{i\epsilon t}{\hbar}}\frac{2^5\sqrt{2}}{3^4}\psi_1(t).$$

Решая полученную систему, получим

$$\psi_2(t) = -ie^{-i\frac{\epsilon}{2}t}\frac{C}{\sqrt{\epsilon^2 + C^2}}\sin\left(\frac{\sqrt{\epsilon^2 + C^2}}{2\hbar}t\right); \qquad C := \frac{2^6\sqrt{2}}{3^4}e\mathcal{E}a.$$

And we have the answer. The probability of being in an excited state:

$$P_{n=2}(T) = \frac{C^2}{\epsilon^2 + C^2}\sin^2\left(\frac{\sqrt{\epsilon^2 + C^2}}{2\hbar}T\right)$$

The probability of remaining in the ground state:

$$P_{n=1}(T) = 1 - \frac{C^2}{\epsilon^2 + C^2}\sin^2\left(\frac{\sqrt{\epsilon^2 + C^2}}{2\hbar}T\right)$$

ПТФ-8.з2. Landau-Zener problem by PT

Рассмотрим произвольную двухуровневую систему, описываемую волновой функцией $|\psi(t)\rangle = \begin{pmatrix}\psi_1(t)\\ \psi_2(t)\end{pmatrix}$ и следующим гамильтонианом, зависящим от времени: $\hat{H}(t) = \begin{pmatrix}\alpha t & \gamma\\ \gamma & -\alpha t\end{pmatrix}$. В начальный момент времени $t \to -\infty$, система находилась в первом состоянии (так что $|\psi_1(t \to -\infty)|^2 = 1$). Определите вероятность перехода системы во второе состояние после такой эволюции $|\psi_2(t \to \infty)|^2$, считая «скорость движения уровней» большой $\alpha \gg \gamma^2$.

Solution.

Выделим в гамильтониане невозмущённую и возмущённую части:

$$\hat{H}(t) = \hat{H}_0(t) + \hat{V}(t), \qquad \hat{H}_0(t) = \begin{pmatrix}\alpha t & 0\\ 0 & -\alpha t\end{pmatrix}, \qquad \hat{V} = \begin{pmatrix}0 & \gamma\\ \gamma & 0\end{pmatrix}$$

Эволюция состояний, если бы не было возмущения ($\gamma = 0$):

$$i\hbar\frac{\partial|\psi_1(t)\rangle}{\partial t} = \alpha t|\psi_1\rangle, \quad i\hbar\frac{\partial|\psi_2(t)\rangle}{\partial t} = -\alpha t|\psi_2\rangle$$

$$|\psi_1(t)\rangle = \exp\left(-i\frac{\alpha t^2}{2\hbar}\right)|\psi_1\rangle \qquad |\psi_2(t)\rangle = \exp\left(i\frac{\alpha t^2}{2\hbar}\right)|\psi_2\rangle,$$

Нестационарная теория возмущений:

$$i\hbar\frac{\partial\psi_2(t)}{\partial t} = V_{21}\psi_1(t), \quad V_{21} = \langle\psi_2(t)|\hat{V}|\psi_1(t)\rangle$$

$$V_{21} = \gamma\exp\left(-i\alpha t^2/\hbar\right)$$

It is really important that here we take matrix element with time-dependent wavefunctions.

$$i\hbar\frac{\partial\psi_2(t)}{\partial t} = \gamma\exp\left(-i\alpha t^2/\hbar\right)\psi_1(t) \approx \gamma\exp\left(-i\alpha t^2/\hbar\right)$$

This approximation is taken because anyway we know that the probability is little.

$$\psi_2(t \to \infty) = -\frac{i\gamma}{\hbar}\int\limits_{-\infty}^{\infty}\exp\left(-i\alpha t^2/\hbar\right)dt = \frac{\sqrt{\pi i}\gamma}{\sqrt{\alpha}\hbar}$$

(??? check $\hbar$ by dimensions????)
Вероятность перехода системы во второе состояние:

$$P = \frac{\pi\gamma^2}{\alpha\hbar^2}$$

ПТФ-8.з3. Осциллятор

Consider an electron moving in a harmonic oscillator and in an electric field that changes with time.:

$$\hat{H}(t) = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2} + e\mathcal{E}(t)\hat{x}, \quad \mathcal{E}(t) = \mathcal{E}_0 e^{-\frac{t^2}{\tau^2}}$$

At $t \to -\infty$, the electron is in the ground state of the system. Determine the probability of detecting it in an arbitrary n-th excited state at $t \to +\infty$ in the leading order of perturbation theory (considering the field weak $e^2\mathcal{E}^2 \ll m\omega^3$).

Solution.

this needs to be think again!!!

Эволюция состояний, если бы не было возмущения:

$$|n(t)\rangle = e^{-i\omega(n+\frac{1}{2})t}|n(0)\rangle$$

$$V_{nm}(t) = -e\mathcal{E}_0 e^{-\frac{t^2}{\tau^2}}\langle n(t)|x|m(t)\rangle = -\frac{e\mathcal{E}_0 e^{-\frac{t^2}{\tau^2}}}{\sqrt{2m\omega}}\begin{cases} e^{i\omega t}\sqrt{n}, & m = n-1 \\ e^{-i\omega t}\sqrt{n+1}, & m = n+1 \end{cases}$$

n-ый порядок теории возмущений:

$$i\hbar\frac{\partial\psi_n(t)}{\partial t} = V_{nn-1}\psi_{n-1}(t) = -\frac{e\mathcal{E}_0 e^{-\frac{t^2}{\tau^2}}e^{i\omega t}}{\sqrt{2m\omega}}\sqrt{n}\psi_{n-1}(t)$$

$$\psi_n(t\to\infty) = \left(\frac{ie\mathcal{E}_0}{\hbar\sqrt{2m\omega}}\right)^n\sqrt{n!}\int\limits_{-\infty}^{\infty}d\tau_1 e^{-\frac{\tau_1^2}{\tau^2}+i\omega\tau_1}\int\limits_{-\infty}^{\tau_1}d\tau_2 e^{-\frac{\tau_2^2}{\tau^2}+i\omega\tau_2}...\int\limits_{-\infty}^{\tau_{n-1}}d\tau_n e^{-\frac{\tau_n^2}{\tau^2}+i\omega\tau_n}$$

Эти интегралы можно превратить в интеграл по всему $\mathbb{R}^n$, разделив на 2^{n-1}:

$$\psi_n(t\to\infty) = 2^{1-n}\left(\frac{ie\mathcal{E}_0}{\hbar\sqrt{2m\omega}}\right)^n\sqrt{n!}\int\limits_{\mathbb{R}^n}dt^n e^{-\frac{t^2}{\tau^2}}e^{i\omega\sum\limits_{i=1}^{n}t_i} = \frac{2}{\sqrt{n!}}\left(\frac{ie\mathcal{E}_0\sqrt{\pi}\tau e^{-\frac{\omega^2\tau^2}{4}}}{2\hbar\sqrt{2m\omega}}\right)^n$$

Вероятность оказаться в n-том состоянии:

$$P_n = \frac{4}{n!}\left(\frac{e^2\mathcal{E}_0^2\pi\tau^2 e^{-\frac{\omega^2\tau^2}{2}}}{8m\hbar^2\omega}\right)^n$$

(?? не очень понимаю, там Планк в знаменателе, от этого не будет ли большая вероятность? не должна быть, но из формулы это не очень видно)

ПТФ-8.з.4. Two-photon ionization (??????)

Fermi's golden rule is typically used to calculate the ionization intensity of a bound state in a one-dimensional delta well $U(x) = -\frac{\kappa}{m}\delta(x)$. Did the problem have an ionization threshold ? - in particular, when $\omega < E_0 = \frac{\kappa^2}{2m}$, the answer was zero. Of course, the reason for this is the use of first-order perturbation theory ('single-photon approximation"); the real answer is nonzero at all frequencies. In this task, it is proposed to investigate, how is the generalization of Fermi's golden rule based on the example of the same problem at frequencies $\frac{E_0}{2} < \omega < E_0$, where two-photon processes provide the leading contribution.

a) Derive a second-order correction of perturbation theory for a harmonic perturbation of the general form $\hat{V}(t) = \hat{F}e^{-i\omega t} + \hat{F}^\dagger e^{i\omega t}$ to an arbitrary coefficient $a_f(t)$, assuming that the particle was originally located in some state of the $|\psi_i\rangle$ discrete spectrum. The structure of the response allows for the following interpretation: the transition occurs first in a virtual way to a certain intermediate level of $i \to \nu$, and then ? - to the final state of $\nu \to f$. Note that the intermediate state of ν, generally speaking, refers to a continuous spectrum.

b) The resulting expression contains quite a lot of terms, having different interpretations, the time-dependent parts in the limit of $t \to \infty$ will turn into a delta function of a certain type. Given the absence of single-photon processes ($\omega < E_0$), demonstrate, that the contribution in the limit of $t \to \infty$ will be from only one member. Based on this, write out an analogue of Fermi's golden rule for this task.

c) Calculate the necessary matrix elements of transitions from the initial state to the intermediate state $F_{i\nu}$ and from the intermediate to the final state $F_{\nu f}$. Because as an intermediate, Similarly, the final states belong to a continuous spectrum., then the corresponding integral, formally speaking, diverges. To determine it, use, for example, the exponential regularization of $e^{-\alpha|x|}$, considering the limit of $\alpha \to 0$.

d) Calculate the necessary integral over the intermediate states of $d\nu$. If we use the matrix element from the previous paragraph at $\alpha \equiv 0$, The corresponding integral, generally speaking, will diverge, since it will contain a pole on the real axis. However, an arbitrarily small $\alpha \to 0$ will shift this pole into a complex plane, making it possible to calculate the integral using the deduction theorem. Finally, using the generalization of Fermi's golden rule derived in the second paragraph, write, how the probability of ionization works as a function of frequency. Express the answer in terms of the frequency ω, the energy of the bound state in the well E_0, and the mass m, the charge e and the amplitude of the electric field $\mathcal{E}$. Construct the answer numerically.

Solution. а)

(решения нет и пока не думал о ней)

Solution. б)

Solution. с)

Solution. д)

17.1.5 Problems about Time-Dependent PT 2

ФР. Переход в колодце под $\hat{V} = F_0 x^3 \frac{1}{1+t^2/\tau^2}$

На заряженную частицу, находящейся в бесконечно глубокой потенциальной яме шириной $a(0 < x < a)$, действует внешнее возмущение $\hat{V} = \mathrm{F_0 x^3} \frac{1}{1+\mathrm{t}^2/\tau^2}$. Считая, что до включения возмущения $(t \to -\infty)$ частица находилась в n-м возбужденном состоянии, найти в первом порядке теории возмущений вероятность его спонтанного перехода в основное состояние $(t \to \infty)$.

Solution.

(??? тут фигня какая-то, все нужно переписать!!!)

$$I = \int_a^a \sin\left(\frac{nx}{a}\right) \sin\left(\frac{\pi n x}{a}\right) x^3 dx = \int_0^{a_0^0} \frac{1}{2} \cos\left(\frac{\pi x}{a} - \frac{\pi n x}{a}\right) x^3 dx - \int_0^a \frac{1}{2} \cos\left(\frac{\pi n x}{a} + \frac{\pi x}{a}\right) x^3 dx$$

$$\int_0^a \cos\left(\frac{\Delta \pi x}{a}\right) x^3 dx = \frac{a^4}{A^4 \pi^4} \left\{6 + 3\left(-2 + \Delta^2 \pi^2\right) \cos(A\pi) + A\pi \left(A^2 \pi^2 - 6\right) \sin(A\pi)\right\}, n_0 \neq 0$$

Вычисление интегралов на wolfram (???)

(??? вроде какие-то у вольфрама проблемы с этим???)

Г-8.47. Внезапно

Система, описываемая гамильтонианом $\hat{H}_\mathbf{0}$, находится в n-м стационарном состоянии дискретного спектра. При $t = 0$ гамильтониан системы внезапно изменяется и становится равным (при $t > 0$) $\hat{H}_f = \hat{H}_0 + \hat{V}_0$, где $\hat{V}_0$, как и $\hat{H}_0$, от времени не зависят. Найти вероятности различных стационарных состояний системы при $t > 0$. Каково среднее значение энергии, приобретаемой системой? Показать, что в случае малого возмущения $\hat{V}_0$ установленные результаты могут быть получены также в рамках нестационарной теории возмущений.

Г-8.48. Переходы при внезапном воздействии дельта импульсом

Система подвергается импульсному воздействию $\hat{V} = \hat{W}_0 \delta(t)$, так что ее гамильтониан имеет вид $\hat{H} = \hat{H}_0 + \hat{W}_0 \delta(t)$. При $t < 0$ система находилась в n-м состоянии дискретного спектра. Найти вероятности различных квантовых состояний при $t > 0$. В случае $\hat{W}_0 = -xP_0$ дать наглядную интерпретацию полученного результата. Сравнить его для малого возмущения $\hat{V}$ с результатом нестационарной теории возмущений.

8.48. Для определения измеления волновой функции под влиянием импульсного воздействия его удобно рассматривать как предельный переход при $\tau \to 0$ взаимодействия вида $\nabla(t, \tau) = \tilde{W}_0 f(t)$, где функция $f(t)$ отлична от нуля лишь при $|t| < \tau$, Шрёдингера при $|t| < \tau$ принимает вид $i\hbar\dot{\Psi} = \hat{W}_0 f(t)\Psi$ (слагаемое $\hat{H}_0$ в гамильтониане опущено, так как оно не дает изменения в. ф. за бесконечно малый промежуток времени τ; в учтенном же слагаемом при этом $f(t) \sim 1/\tau \to \infty$). Решение этого уравнения

$$\Psi(t) = \exp\left(-\frac{i}{\hbar} \int_{-\tau}^{t} f\left(t'\right) dt' \hat{W}_0\right) \Psi(-\tau).$$

Положив здесь $t = \tau$ и устремляя $\tau \to 0$, находим искомое изменение волновой функции

$$\Psi(t = 0+) = \exp\left(-i\hat{W}_0/\hbar\right)\Psi(t = 0-).$$

Учитывая, что по условию задачи $\Psi(0-) = \Psi_n^{(0)}$, находим искомые вероятности

$$w(n \to k) = |\int \Psi_k^{(0)*} \exp\left(-\frac{i}{\hbar}\hat{W}_0\right)\Psi_n^{(0)} d\tau_q|^2.$$

Разложение экспоненты в ряд в случае малого возмущения, когда $|\,(\mathscr{W}_0)_{kn}\,| \ll \hbar$, дает

$$w^{(1)}(n \to k) = \frac{1}{\hbar^2}|\left(\hat{W}_0\right)_{kn}|^2, \quad k \neq n$$

что совпадает с результатом нестационарной теории возмущений, получающимся непосредственным (благодаря δ-функции) интегрированием в формуле (VIII.8).

Воздействие вида $V(x,t) = -xP_0\delta(t)$ на классическую частицу состоит в мгновенной передаче ей импульса $P_0 = \int F(t)dt$. Это утверждение остается справедливым и в квантовой механике, что следует из формулы (2). Действительно, в. ф. состояний частицы в импульсном представлении непосредственно до: $a_i(p) = \langle p|t = 0-\rangle$, и сразу после: $a_f(p) = \langle p|t = 0+\rangle$, воздействия связаны соотношением $a_f(p) = a_i\,(p - P_0)$, что и отражает отмеченное выше обстоятельство об изменении импульса частицы.

Г-8.49. Внезапно

Частица находится в основном состоянии в бесконечно глубокой потенциальной яме шириной a ($0 < x < a$). В некоторый момент времени правая стенка ямы за короткий интервал времени τ смещается в точку $b > a$. Найти вероятности возбуждения различных квантовых состояний частицы после остановки стенки.

Г-8.50. Внезапно

Частица находится в основном состоянии в δ-яме, так что $U = -\alpha\delta(x)$. Внезапно параметр α, характеризующий «глубину» ямы, изменяется и становится равным $\tilde{\alpha}$ (сравнить с изменением заряда ядра атома, например, при β-распаде). Найти

Г-8.52. Переходы при внезапном наложение поля на осциллятор

На заряженный осциллятор, находящийся в основном состоянии, внезапно накладывается однородное электрическое поле, направленное вдоль оси колебаний. Найти вероятности возбуждения различных состояний осциллятора после включения поля. Сравнить с результатом задачи 6.25.

Solution.

Для решения задачи важно понимать решение задачи о резком изменении гамильтониана $\hat{H}_0$ с дискретным спектром, который внезапно становится равным $\hat{H}_f = \hat{H}_0 + \hat{V}_0$, где $\hat{V}_0$, как и $\hat{H}_0$ от времени не зависят. В этой задаче важно видеть, что коэффициенты в разложении в. ф. $\Psi_{n,i}$ по с. ф. $\Psi_{k,f}$ конечного гамильтониана $\left(H_f = H_0 + \hat{V}_0\right)$,

$$\Psi_{n,i} = \sum_k c_{kn}\Psi_{k,f},$$

определяют искомые вероятности перехода:

$$w(n \to k) = |c_{kn}|^2 = |\langle k, f|n, i\rangle|^2.$$

В этих же обозначениях и будем решать эту задачу.

Воспользуемся формализмом операторов рождения и уничтожения $\hat{a}^+, \hat{a}$. Для невозмущенного осциллятора $\hat{a}_i = (2\hbar)^{-1/2}(\lambda x + i\lambda^{-1}\hat{p})$, где $\lambda = \sqrt{m\omega}$; при этом его основное состояние определяется соотношением $\hat{a}_i|0, i\rangle = 0$. Наложение электрического поля эквивалентно смещению точки равновесия осциллятора на расстояние $x_0 = e\mathscr{E}/m\omega^2$, так что теперь $\hat{a}_f = \hat{a}_i - \lambda(2\hbar)^{-1/2}x_0$, а конечные (при $t > 0$, после наложения поля) стационарные состояния определяются соотношениями

$$|n, f\rangle = \frac{1}{\sqrt{n!}}\left(\hat{a}_f^+\right)^n|0, f\rangle, \quad \hat{a}_f|0, f\rangle = 0.$$

Найдем коэффициенты c_n. Подействовав на обе части $|0,i\rangle = \sum\limits_n c_n|n,f\rangle$ оператором $\hat{a}_{in}$ и учтя, что $\hat{a}(t) = e^{-i\omega t}\hat{a}_i$ при $t \to -\infty$, а также соотношение

$$\hat{a}_f|n,f\rangle = \sqrt{n}|n-1,f\rangle,$$

приходим к рекуррентному соотношению $c_n = (\alpha/\sqrt{n})c_{n-1}$. Из него следует, что $c_n = \left(\alpha^n/\sqrt{n!}\right)c_0$. При этом условие нормировки

$$\langle 0,\ \mathrm{i}\ |0,\ \mathrm{i}\ \rangle = \sum_n |c_n|^2 = 1$$

дает

$$|c_0|^2 = \exp\left(-|\alpha|^2\right).$$

Вероятности переходов:

$$w(0 \to n) = |c_n|^2 = \frac{1}{n!}\alpha^{2n}e^{-\alpha^2}, \quad a = -\frac{\lambda x_0}{\sqrt{2\hbar}}.$$

Видно, что зависимость вероятностей от номера n квантового состояния осциллятора описывается распределением Пуассона.

ФР-кр-3-курс.1.(???)

Частица массы m движется в одномерной потенциальной яме вида рис.1.

$$U(x) = \begin{cases} \infty, & x < 0, \\ 0, & (0 < x < a), \\ v_0, & x > a. \end{cases}$$

При каких соотношениях между a и v_0 в этой яме имеются 4 дискретные уровни.

(??? тут типичные задачи контрольной, которые нужно научиться решать, я все еще не научился, потому что забил. плохо, нужно тренироваться!!!!! уже мб похожее и вписано, если так, то удалю их тут потом)

ФР-кр-3-курс.2.(???)

Частица находится в основном состоянии линейного гармонического осциллятора. Найти вероятность пребывания этой частицы в области, запрещенной для классического движения.

ФР-кр-3-курс.3.(???)

Состояние частицы, находящейся в бесконечно глубокой потенциальной яме шириной $a(0 < \mathrm{x} < a)$ описывается волновой функцией вида:

$$\Psi(\mathrm{x}) = c\sin^3(\pi \mathrm{x}/a).$$

Найти распределение вероятностей различных значений энергий.

ФР-кр-3-курс.4.(???)

Угловая часть ВФ частицы в центральном поле имеет вид $\Phi(\theta,\varphi) = C\cos^2\theta$. Найти вероятности различных значений момента частицы и среднее значение квадрата момента.

ФР-кр-3-курс.5.(???)

Состояние плоского ротатора описывается волновой функцией вида $\Psi = A\sin(2\varphi)$. Найти функции распределения ротатора по энергиям и проекциям момента, а также средние значения этих величин в указанном состоянии.

ФР-кр-3-курс.6.(???)

Для основного состояния частицы в бесконечно глубокой сферической потенциальной яме:

$$\mathrm{U(r)} = \begin{cases} 0, & r \le a \\ \infty, & r > a \end{cases}$$

найти $\langle \mathrm{r} \rangle$.

ФР-кр-3-курс.7.(???)

Покажите, что среднее значение $\langle \mathrm{r}^{-3} \rangle$ для 3 d волновой функции водородоподобного атома равно $27z^3/15a^3$.

17.1.6 Problems about adiabatics 1: Fun Models

ПТФ-9.у1. Ионизация

Имеется двухъямный потенциал $U(x) = -\frac{\kappa}{m}\left[\delta(x+\frac{L(t)}{2}) + \delta(x-\frac{L(t)}{2})\right]$. В начальный момент времени ямы разнесены друг от друга бесконечно далеко, $L \to \infty$, и электрон находится в одной из ям. Расстояние между ямами затем меленно уменьшается до нуля, так что в какой-то момент времени две ямы сливаются в одну: $U(x) = -\frac{2\kappa}{m}\delta(x)$. Определите, с какой вероятностью электрон останется в яме в результате такого процесса.

Solution.

Воспользуемся решением 3 задачи 3 недели. При $L \to \infty$ реализуется туннельный режим. Волновая функция электрона в начальный момент времени:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(\psi_{\text{чёт}} + \psi_{\text{нечет}})$$

где $\psi_{\text{чёт}}$ – чётная волновая функция, $\psi_{\text{нечет}}$ – нечётная. Нечётное состояние существует только при $\kappa L \geq 1$. Поэтому при $L \to 0$ выживет только чётное связанное состояние, нужно узнать вероятность нахождения электрона в нём. По адиабатической теореме в процессе, состояние частицы в произвольный момент времени электрон будет оставаться в состоянии той чётности, в котором он оказался в начальный момент.

$$\psi_{\text{чёт}}(t) \propto \frac{1}{\sqrt{2}}\psi_{\text{чёт}}(0)$$

Вероятность остаться в яме:

$$P = \frac{1}{2}$$

ПТФ-9.у2. Адиабатика для колебаний ямы

Частица массы m движется в бесконечно глубокой потенциальной яме ширины $a(t)$, которая меняется во времени согласно следующему закону:

$$a(t) = a(1 - \alpha \sin^2 \omega t), \quad \alpha < 1$$

При каких условиях в такой задаче следует ожидать применимость адиабатического приближения?

Solution.

Уровни энергии в бесконечно глубокой яме:

$$E_n = \frac{\pi^2\hbar^2 n^2}{2ma^2}$$

$$\Delta E = E_{n+1} - E_n = \frac{\pi^2\hbar^2(2n+1)}{2ma^2} \geq \frac{\pi^2\hbar^2}{2ma^2}$$

Критерий адиабатичности:

$$\omega \ll \Delta E$$

Таким образом, условия применимости адиабатичности:

$$\frac{\pi^2\hbar^2}{2ma^2} \gg \omega$$

ПТФ-9.з1. Переворот спина

Спин-1/2 находится в магнитном поле $\vec{B}$, которое медленно вращается в плоскости yz:

$$\hat{H} = -\mu\vec{B}\cdot\hat{\vec{\sigma}}, \quad \vec{B}(t) = B\left(0, \frac{1}{\cosh\omega t}, -\tanh\omega t\right)$$

и $\omega \ll \mu B$. В начальный момент времени $t \to -\infty$ спин и магнитное поле направлены по оси z. Найдите в первом неисчезающем порядке вероятность того, что спин останется направленным по оси z после завершения вращения при $t \to \infty$.

Solution.

$$\hat{H} = -\mu\vec{B}\cdot\hat{\vec{\sigma}} = -\mu\begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix} = \mu B\begin{pmatrix} \tanh\omega t & \frac{i}{\cosh\omega t} \\ -\frac{i}{\cosh\omega t} & -\tanh\omega t \end{pmatrix}$$

Собственные значения и векторы этой матрицы:

$$E_- = -\mu B, \quad E_+ = \mu B$$

$$|\psi_-\rangle = \frac{1}{\sqrt{1+e^{-2\omega t}}}\begin{pmatrix} -ie^{-\omega t} \\ 1 \end{pmatrix}, \quad |\psi_+\rangle = \frac{1}{\sqrt{1+e^{2\omega t}}}\begin{pmatrix} ie^{\omega t} \\ 1 \end{pmatrix}$$

В начальный момент $c_- = 1$, $c_+ = 0$. Нестационарная адиабатика:

$$c_+(T\to\infty) = \int\limits_{-\infty}^{\infty} \exp\left(i\int\limits_0^t \omega_{+-}(\tau)d\tau\right)\frac{\langle\psi_+|\partial_t\hat{H}|\psi_-\rangle}{\omega_{+-}(t)}dt, \quad \omega_{+-} = E_+ - E_- = 2\mu B$$

$$\partial_t\hat{H} = \frac{\mu B\omega}{\cosh^2\omega t}\begin{pmatrix} 1 & -i\sinh\omega t \\ i\sinh\omega t & -1 \end{pmatrix}$$

$$\langle\psi_+|\partial_t\hat{H}|\psi_-\rangle = -\frac{\mu B\omega}{\cosh\omega t}$$

(!!! add the derivation of it here!!!)

$$c_-(T\to\infty) = -\int\limits_{-\infty}^{\infty}\frac{\exp\left(i2\mu Bt\right)}{2\cosh\omega t}\omega dt = -\int\limits_{-\infty}^{\infty}\frac{\exp\left(i\frac{2\mu Bx}{\omega}\right)}{2\cosh x}dx - \frac{\pi}{2\cosh\frac{\pi\mu B}{\omega}}$$

Вычислим интеграл при помощи вычетов. Нули знаменателя: $z_k = \pi i\left(\frac{1}{2}+k\right), k\in\mathbb{Z}$. Берём только полюс $z_0 = \frac{i\pi}{2}$.

$$c_-(T\to\infty) = -2\pi i\operatorname*{res}_{z=\frac{i\pi}{2}}\frac{\exp\left(i\frac{2\mu Bz}{\omega}\right)}{2\cosh z} = -\pi\exp\left(-\frac{\pi\mu B}{\omega}\right)$$

Вероятность того, что спин будет направлен по оси z:

$$P = \pi^2\exp\left(-\frac{2\pi\mu B}{\omega}\right)$$

ПТФ-9.з2. Эффект Ааронова-Бома

The electron can move along the ring of radius R, and is in the bound state of the potential well $U(\varphi) = -U_0\delta(\varphi-\varphi_0)$. A magnetic flux Φ is passed through the ring, so that the Hamiltonian of the system has the form:

$$\hat{H} = \frac{(\hat{p}_\varphi - \frac{e}{c}A_\varphi)^2}{2m} - U_0\delta(\varphi-\varphi_0), \qquad \hat{p}_\varphi = -\frac{i}{R}\frac{\partial}{\partial\varphi}, \qquad A_\varphi = \frac{\Phi}{2\pi R}$$

Then, one slowly moves the delta-potential around the ring clockwise (the value of φ_0 varies from $\varphi_0(0) = 0$ to $\varphi_0(T) = 2\pi$). Determine the dependence of the phase that the electron wave function will receive as a result of such evolution on the energy. Assume, that size of the bound state is much smaller than the radius of the ring.

Solution.

Стационарное уравнение Шрёдингера:

$$\hat{H}\psi(\varphi) = E\psi(\varphi)$$

$$\hat{H} = \frac{(\frac{i}{R}\frac{\partial}{\partial\varphi} + \frac{e\Phi}{2\pi Rc})^2}{2m} - U_0\delta(\varphi-\varphi_0) = -\frac{1}{2mR^2}\partial_\varphi^2 + \frac{ie\Phi}{2\pi R^2 mc}\partial_\varphi + \frac{e^2\Phi^2}{8\pi^2R^2mc^2} - U_0\delta(\varphi-\varphi_0)$$

При $\varphi \neq \varphi_0$:

$$\left(\frac{i}{R}\frac{\partial}{\partial\varphi} + \frac{e\Phi}{2\pi Rc}\right)^2\psi(\varphi) = 2mE\psi(\varphi)$$

Ищем решение $\psi(\varphi)$ в виде экспоненты:

$$\left(\frac{i}{R}\lambda + \frac{e\Phi}{2\pi Rc}\right)^2 = 2mE$$

$$\lambda_{1,2} = i\left(\frac{e\Phi}{2\pi c} \pm \sqrt{2mE}R\right)$$

Поскольку состояние связанное $E<0$, то

$$\lambda_{1,2} = \left(\frac{ie\Phi}{2\pi c} \mp \sqrt{2m|E|}R\right)$$

We introduce

$$A = \frac{e\Phi}{2\pi c}, \qquad B = \sqrt{2m|E|}R.$$

$$\psi(\varphi) = C_1e^{(iA-B)\varphi} + C_2e^{(iA+B)\varphi}$$

Положим $\varphi_0 = 0$, а после сшивки сдивнем φ обратно. Условия сшивки:

$$\begin{cases}\psi(0+0) = \psi(2\pi-0),\\ \psi'(0) - \psi'(2\pi-0) = -2mU_0R^2;\end{cases}$$

(!!!! write math here!!!!)

$$\begin{cases}C_1 + C_2 = C_1e^{(iA-B)2\pi} + C_2e^{(iA+B)2\pi},\\ (iA-B)C_1 + (iA+B)C_2 - (iA-B)C_1e^{(iA-B)2\pi} - (iA+B)C_2e^{(iA+B)2\pi} = -2mU_0R^2(C_1+C_2);\end{cases}$$

Выразим C_2 через C_1:
(!!!! write math here!!!! I think, there is a big problem with math here!!!)

$$C_2 = -C_1e^{-2\pi B}\frac{\sin(\pi(A+iB))}{\sin(\pi(A-iB))}$$

Характерный размер волновой функции $\ll R$, поэтому $e^{-B\varphi} \ll 1$ и $B \gg 1$. Условие нормировки:

$$\int\limits_0^{2\pi}|\psi(\varphi)|^2d\varphi = 1$$

(??? here are problems, I don't know, how to extract these coefficients)
Пользуясь тем, что $B \gg 1$, получим

$$C_2 = \sqrt{B}e^{-2\pi B}, \quad C_1 = \sqrt{B}e^{2\pi iA}$$

$$\psi(\varphi) = \sqrt{B}e^{2\pi iA}e^{(iA-B)\varphi} + \sqrt{B}e^{-2\pi B}e^{(iA+B)\varphi}$$

Сдвигая на угол φ_0, получим

$$\psi(\varphi) = \sqrt{B}e^{2\pi iA}e^{(iA-B)(\varphi-\varphi_0)} + \sqrt{B}e^{-2\pi B}e^{(iA+B)(\varphi-\varphi_0)}$$

Now, we need only to plug this wavefunction in the definition of Barry's phase:

$$\gamma = \int_0^{2\pi} d\varphi_0 \langle \psi(\varphi_0) | i\partial_{\varphi_0} | \psi(\varphi_0) \rangle$$

$$\partial_{\varphi_0}\psi(\varphi_0) = -\sqrt{B}e^{2\pi i A}(iA-B)e^{(iA-B)(\varphi-\varphi_0)} - \sqrt{B}(iA+B)e^{-2\pi B}e^{(iA+B)(\varphi-\varphi_0)}$$

$$\langle \psi(\varphi_0) | i\partial_{\varphi_0} | \psi(\varphi_0) \rangle = -\int_0^{2\pi} d\varphi (\sqrt{B}e^{-2\pi i A}e^{(-iA-B)(\varphi-\varphi_0)} + \sqrt{B}e^{-2\pi B}e^{(-iA+B)(\varphi-\varphi_0)})i$$
$$(\sqrt{B}e^{2\pi i A}(iA-B)e^{(iA-B)(\varphi-\varphi_0)} + \sqrt{B}(iA+B)e^{-2\pi B}e^{(iA+B)(\varphi-\varphi_0)}) = A$$

(!! I'll check math later)

$$\gamma = \int_0^{2\pi} d\varphi_0 A = 2\pi A$$

$$\gamma = \frac{e\Phi}{c}$$

ПТФ-9.з3. Adiabatic rotation of a box

Consider a square two-dimensional box of size $L \times L$ with infinite walls. An arbitrary stationary state can be characterized by two quantum numbers $|n_x, n_y\rangle$, which number the number of nodes x and y components of the wave function; in particular, the states $|1,0\rangle$ and $|0,1\rangle$ have the same energy. Let's assume that at the initial moment of time the wave function was an arbitrary linear combination of the ground states:

$$|\psi(0)\rangle = \psi_1|1,0\rangle + \psi_2|0,1\rangle$$

Here ψ_1, ψ_2 are some complex numbers. Then the box slowly rotates in the plane at an angle of 2π clockwise, so that after rotation its new position coincides with the original one. Determine the wave function $|\psi(T)\rangle$ after such a rotation.

Introduction to solution

Slow rotation is described by a nonstationary adiabatics, where

$$\psi_n(t) \equiv c_n(t) \cdot \exp\left(-i\int_{t_0}^{t} E_n(\tau)d\tau\right),$$

$$c_m(T) \approx \int_{t_0}^{T} \exp\left(i\int_{t_0}^{t}\omega_{mn}(\tau)d\tau\right)\frac{\left\langle m(t)\left|\partial_t\hat{H}\right|n(t)\right\rangle}{\omega_{mn}(t)}dt.$$

$\omega_{nm} = E_n - E_m$.

$$i\partial_\theta c_n(\theta) = -i\sum_m \exp\left(i\int\omega_{nm}(\tau)d\tau\right)\langle n(\theta)|\partial_\theta|m(\theta)\rangle c_m(\theta),$$

Here n is the number of a state in which there is a particle
(???? write a good intro to solutions!!!)

Solution.

This problem is solved by a non-stationary adiabatics. One just need to be careful, use proper equation for the coefficients, do a good approximation and use Wolfram to compute the integrals. The most important part is to consider change of the state only to the ground states and to integrate in formula for adiabatics for the coordinates that correspond to the current position of a box, not the initial one.

Let us assume that the center of coordinates of the box coincides with the center of coordinates of XY system. The wavefunction of a particle in a box is:

$$\psi_{n,m} = \frac{2}{L}\sin\left(k_n\left(x+\frac{L}{2}\right)\right)\sin\left(k_m\left(\frac{L}{2}+y\right)\right)$$

$$|1,0\rangle = \frac{2}{L}\sin\left(\frac{2\pi}{L}\left(x+\frac{L}{2}\right)\right)\sin\left(\frac{\pi}{L}\left(\frac{L}{2}+y\right)\right) = \frac{2}{L}\sin\left(\frac{2\pi}{L}x\right)\cos\left(\frac{\pi}{L}y\right),$$
$$|0,1\rangle = \frac{2}{L}\sin\left(\frac{\pi}{L}\left(x+\frac{L}{2}\right)\right)\sin\left(\frac{2\pi}{L}\left(\frac{L}{2}+y\right)\right) = \frac{2}{L}\sin\left(\frac{2\pi}{L}y\right)\cos\left(\frac{\pi}{L}x\right)$$

Here we neglected minus from $\sin(x+\pi) = -\sin(x)$, because anyway the result will be the same.

By rotation we mean that coordinates are changed as:

$$\begin{cases} x_\theta = x\cos\theta - y\sin\theta, \\ y_\theta = x\sin\theta + y\cos\theta. \end{cases}$$

Thus, the bases vectors will change as

$$|1,0\rangle = \frac{2}{L}\sin\left(\frac{2\pi}{L}x_\theta\right)\cos\left(\frac{\pi}{L}y_\theta\right),$$

$$|0,1\rangle = \frac{2}{L}\sin\left(\frac{2\pi}{L}y_\theta\right)\cos\left(\frac{\pi}{L}x_\theta\right).$$

It is important to work with for instance x_θ, and not with the full its expression, because otherwise the expressions will be incomprehensible big. Now we use the framework of the non-stationary adiabatics, in which

$$\partial_\theta c_n(\theta) = -\sum_{m=|0,1\rangle,|1,0\rangle} \langle n(\theta)|\partial_\theta|m(\theta)\rangle c_m(\theta)$$

This is the consequence of the general formula $i\partial_\theta c_n(\theta) = -i\sum\limits_m \exp\left(i\int\omega_{nm}(\tau)d\tau\right)\cdot\cdot\langle n(\theta)|\partial_\theta|m(\theta)\rangle c_m(\theta)$, were $\omega_{nm} = E_n - E_m = 0$ because we have here only the ground states, which have the same energy (they give the biggest contribution).

Or, explicitly, we have:

$$\partial_\theta c_1(\theta) = -\langle 1,0|\partial_\theta|1,0\rangle c_1(\theta) - \langle 1,0|\partial_\theta|0,1\rangle c_2(\theta)$$
$$\partial_\theta c_2(\theta) = -\langle 0,1|\partial_\theta|1,0\rangle c_1(\theta) - \langle 0,1|\partial_\theta|0,1\rangle c_2(\theta)$$

Now, we compute from expressions of the basis vectors. First, we note that $dx_\theta/d\theta = -y_\theta$ and $dy_\theta/d\theta = +x_\theta$. Then, we compute

$$\begin{aligned}\partial_\theta|0,1\rangle &= \partial_\theta\left[\frac{2}{L}\sin\left(\frac{2\pi}{L}y_\theta\right)\cos\left(\frac{\pi}{L}x_\theta\right)\right] = \\ &= \frac{2}{L}\left[\cos\left(\frac{2\pi}{L}y_\theta\right)(+\frac{2\pi}{L}x_\theta)\cos\left(\frac{\pi}{L}x_\theta\right) - \sin\left(\frac{2\pi}{L}y_\theta\right)\sin\left(\frac{\pi}{L}x_\theta\right)(-\frac{\pi}{L}y_\theta)\right] = \\ &= \frac{2\pi}{L^2}\left[2\cos\left(\frac{2\pi}{L}y_\theta\right)x_\theta\cos\left(\frac{\pi}{L}x_\theta\right) + \sin\left(\frac{2\pi}{L}y_\theta\right)\sin\left(\frac{\pi}{L}x_\theta\right)y_\theta\right].\end{aligned}$$

Then

$$\langle 0,1|\partial_\theta|0,1\rangle = \int dx_\theta dy_\theta \frac{2}{L}\frac{4\pi}{L^2}\sin\left(\frac{2\pi}{L}y_\theta\right)\cos\left(\frac{\pi}{L}x_\theta\right)\left[2\cos\left(\frac{2\pi}{L}y_\theta\right)x_\theta\cos\left(\frac{\pi}{L}x_\theta\right) + \sin\left(\frac{2\pi}{L}y_\theta\right)\sin\left(\frac{\pi}{L}x_\theta\right)y_\theta\right] = 0.$$

The integration over dx_θ is the manifestation of our main philosophy of adiabatic method, that at each time we consider box as stationary.

(???? think more about this! why is it so? write better theory, that states that this is the meaning of the terms of th r.h.s. of the equation for coefficients.)

(??? do the integral analytically)

Currently the proof is by Wolfram:

```
Integrate[
Sin[2 Pi/L y] Cos[Pi/L x] (2Cos[(2 Pi)/L y] x Cos[Pi/L x] + Sin[(2 Pi)/L y] y Sin[Pi/L x]),
    {x, -L/2, L/2}, {y, -L/2, L/2}]
```

Now, it is clear, what is going on with other factors:

$$\partial_\theta|1,0\rangle = \partial_\theta\left[\frac{2}{L}\sin\left(\frac{2\pi}{L}x_\theta\right)\cos\left(\frac{\pi}{L}y_\theta\right)\right] =$$
$$= \frac{2}{L}\left[\cos\left(\frac{2\pi}{L}x_\theta\right)(-\frac{2\pi}{L}y_\theta)\cos\left(\frac{\pi}{L}y_\theta\right) - \sin\left(\frac{2\pi}{L}x_\theta\right)\sin\left(\frac{\pi}{L}y_\theta\right)(+\frac{\pi}{L}x_\theta)\right] =$$
$$= -\frac{2\pi}{L^2}\left[2\cos\left(\frac{2\pi}{L}x_\theta\right)y_\theta\cos\left(\frac{\pi}{L}y_\theta\right) + \sin\left(\frac{2\pi}{L}x_\theta\right)\sin\left(\frac{\pi}{L}y_\theta\right)x_\theta\right].$$

Thus

$$\langle 1,0|\partial_\theta|1,0\rangle = \int dx_\theta dy_\theta \frac{2}{L}\frac{2\pi}{L^2}\sin\left(\frac{2\pi}{L}x_\theta\right)\cos\left(\frac{\pi}{L}y_\theta\right)\left[-2\cos\left(\frac{2\pi}{L}x_\theta\right)y_\theta\cos\left(\frac{\pi}{L}x_\theta\right) - \sin\left(\frac{2\pi}{L}x_\theta\right)\sin\left(\frac{\pi}{L}y_\theta\right)x_\theta\right] = 0.$$

```
Integrate[
Sin[2 Pi/L x] Cos[ Pi/L y] (-2Cos[(2 Pi)/L x] y Cos[Pi/L y] - Sin[(2 Pi)/L x] x Sin[Pi/L
    y]), {x, -L/2, L/2}, {y, -L/2, L/2}]
```

The fact that it is also zero is obvious because this integral is just exactly the same as the one before, but with different labels of x and y.

Now, two more complicated ones:

$$\langle 1,0|\partial_\theta|0,1\rangle = \int dx_\theta dy_\theta \frac{2}{L}\frac{2\pi}{L^2}\sin\left(\frac{2\pi}{L}x_\theta\right)\cos\left(\frac{\pi}{L}y_\theta\right)\left[2\cos\left(\frac{2\pi}{L}y_\theta\right)x_\theta\cos\left(\frac{\pi}{L}x_\theta\right) + \sin\left(\frac{2\pi}{L}y_\theta\right)\sin\left(\frac{\pi}{L}x_\theta\right)y_\theta\right] =$$
$$= \frac{4\pi}{L^3}\frac{64L^3}{27\pi^3} = \frac{256}{27\pi^3}.$$

(??? analytical calculation of the integral?? I think, it will be just boring and long since all integrals will come to the form $\iint dxdyx\cos(x)$, which is trivially taken by parts)

```
Integrate[
Sin[2 Pi/L x] Cos[ Pi/L y] (2Cos[(2 Pi)/L y] x Cos[Pi/L x] + Sin[(2 Pi)/L y] y Sin[Pi/L x]),
    {x, -L/2, L/2}, {y, -L/2, L/2}]
```

$$\langle 0,1|\partial_\theta|1,0\rangle = \int dx_\theta dy_\theta \frac{2}{L}\frac{2\pi}{L^2}\sin\left(\frac{2\pi}{L}y_\theta\right)\cos\left(\frac{\pi}{L}x_\theta\right)\left[-2\cos\left(\frac{2\pi}{L}x_\theta\right)y_\theta\cos\left(\frac{\pi}{L}y_\theta\right) - \sin\left(\frac{2\pi}{L}x_\theta\right)\sin\left(\frac{\pi}{L}y_\theta\right)x_\theta\right] =$$
$$= -\frac{4\pi}{L^3}\frac{64L^3}{27\pi^3} = -\frac{256}{27\pi^3}.$$

(??? analytical calculation of the integral?? I think, it will be just boring and long since all integrals will come to the form $\iint dxdyx\cos(x)$, which is trivially taken by parts)

```
Integrate[
Sin[2 Pi/L x] Cos[ Pi/L y] (-2 Cos[(2 Pi)/L y] x Cos[Pi/L x] - Sin[(2 Pi)/L y] y Sin[Pi/L
    x]), {x, -L/2, L/2}, {y, -L/2, L/2}]
```

Totally, we have:

$$\langle 1,0|\partial_\theta|1,0\rangle = \langle 0,1|\partial_\theta|0,1\rangle = 0, \quad \langle 1,0|\partial_\theta|0,1\rangle = -\langle 0,1|\partial_\theta|1,0\rangle = \frac{256}{27\pi^2}$$

And equations for the dynamical phase will give us

$$\partial_\theta c_1(\theta) = -\frac{256}{27\pi^2}c_2(\theta), \quad c_1(0) = \psi_1$$
$$\partial_\theta c_2(\theta) = \frac{256}{27\pi^2}c_1(\theta), \quad c_2(0) = \psi_2,$$

We combine these two equations into the second order linear differential equation and the solution of it is

$$c_1(\theta) = \psi_1 \cos\left(\frac{256\theta}{27\pi^2}\right) - \psi_2 \sin\left(\frac{256\theta}{27\pi^2}\right)$$
$$c_2(\theta) = \psi_1 \sin\left(\frac{256\theta}{27\pi^2}\right) + \psi_2 \cos\left(\frac{256\theta}{27\pi^2}\right)$$

The coefficients here are obtained by usual matching boundary conditions $c_1(0) = \psi_1, c_2(0) = \psi_2$.

Thus, for the whole rotation, one just need to plug 2π:

$$\begin{aligned}|\psi(T)\rangle &= c_1(2\pi)|1,0\rangle + c_2(2\pi)|0,1\rangle \\ &= \left(\psi_1 \cos\left(\frac{512\theta}{27\pi}\right) - \psi_2 \sin\left(\frac{512\theta}{27\pi}\right)\right)|1,0\rangle + \left(\psi_1 \sin\left(\frac{512\theta}{27\pi}\right) + \psi_2 \cos\left(\frac{512\theta}{27\pi}\right)\right)|0,1\rangle\end{aligned}$$

This is how our wavefunction will change.

Solution in different coordinates

(??? one can introduce zero of coordinates not in the center of the box, but in the edge. Maybe I'll comment about it, currently, I didn't try this yet)

Solution by Hamiltonian

(???? I don't know, is it possible to write the Hamiltonian of the system and use another formula for the adiabatics? maybe it is possible, since the formulas are equivalent. I'll try later)

What happens with the energy of the system?

(???? a good question, currently, I have no idea. Does the system observe the energy?)

Limits of applicability of the solution

(???? a good question, I first need to write this in the theory)
(?? how many rotations can be done for the system to change the state to the excited state? I think, the adiabatic approximation which is written here should be just rewritten with also other states for m index. So, maybe it is not a trivial problem, I don't know....)

Connection to Berry's phase

(??? can one solve it by Berry's phase??? maybe this is the exactly it, what we are calculating???)

Why does the particle at all will feel the rotation?

If there is no inertia force, then particle will not feel rotation at all.
(???? this is why I think this problem is just broken. the solution above is maybe even generally wrong.)

17.1.7 Problems about adiabatics 2: Template Models

ПТФ-6.пр.1 Landau-Zener problem by adiabatics

Suppose we have a two-level system, where level spacing is changed in time and models by a Hamiltonian

$$\hat{H}(t) = \begin{pmatrix} \alpha t & \gamma \\ \gamma & -\alpha t \end{pmatrix}.$$

Here α and γ are constants.

Find a probability of transfer to the lower state at $t \to \infty$ from the upper one, on which a particle was initially (in time $t \to -\infty$).

Solution

This is the basic example for non-stationary adiabatic methods.

First of all, we compute the energy levels exactly as:

$$E_+(t) = \sqrt{\gamma^2 + (\alpha t)^2}, \quad |\psi_+(t)\rangle = \frac{1}{\sqrt{2\left(\gamma^2 + (\alpha t)^2 + \alpha t\sqrt{\gamma^2 + (\alpha t)^2}\right)}} \begin{pmatrix} \alpha t + \sqrt{\gamma^2 + (\alpha t)^2} \\ \gamma \end{pmatrix}$$

$$E_-(t) = -\sqrt{\gamma^2 + (\alpha t)^2}, \quad |\psi_-(t)\rangle = \frac{1}{\sqrt{2\left(\gamma^2 + (\alpha t)^2 - \alpha t\sqrt{\gamma^2 + (\alpha t)^2}\right)}} \begin{pmatrix} \alpha t - \sqrt{\gamma^2 + (\alpha t)^2} \\ \gamma \end{pmatrix}$$

It is convenient to perametrise them by $\alpha t = \gamma \sinh\theta$

$$E_+(\theta) = \gamma \operatorname{ch}\theta, \quad |\psi_+(\theta)\rangle = \tfrac{1}{\sqrt{2\operatorname{ch}\theta}} \begin{pmatrix} e^{\theta/2} \\ e^{-\theta/2} \end{pmatrix}$$
$$E_-(\theta) = -\gamma \operatorname{ch}\theta, \quad |\psi_-(\theta)\rangle = \tfrac{1}{\sqrt{2\operatorname{ch}\theta}} \begin{pmatrix} e^{-\theta/2} \\ -e^{\theta/2} \end{pmatrix}$$

Initially, at $t \to -\infty$ there was $|\psi_+(-\infty)| = 1$ and $|\psi_-(-\infty)| = 0$; The probability of the transition is

$$P = |\psi_-(+\infty)|^2.$$

(??? why?????)

Сразу выделим параметр адиабатичности.

Если уровни находятся достаточно далеко по энергии, то переходов не будет - поэтому масштаб времени T, который входит в критерий адиабатичности, определяется из условия достаточной близости уровней: $\alpha T \sim \gamma \to T \sim \frac{\gamma}{\alpha}$. С другой стороны, масштаб расстояния между уровнями при этом равен γ. Поэтому адиабатическое приближение соответствует случаю, когда $\gamma^2 \gg \alpha$.

Now, again we use that very non-trivial non-stationary adiabatics. Решая уравнение (6.4) методом последовательных приближений, и в качестве нулевого приближения беря $c_+^{(0)}(t) = 1 = \text{const}$ и $c_-^{(0)}(t) = 0$, в первом приближении мы получаем следующее уравнение на $c_-^{(1)}(t)$, которое, в свою очередь, тривиально интегрируется; наконец, в интеграле удобно перейти опять вместо интегрирования по времени к интегрированию по вспомогательному параметру θ:

$$i\frac{dc_-(t)}{dt} = -ie^{-i\int_0^t \omega_{+-}(\tau)d\tau} \frac{\langle\psi_-(\theta)|\frac{\partial\hat{H}}{\partial\theta}|\psi_+(\theta)\rangle}{\omega_{-+}(\theta)} \cdot \frac{d\theta}{dt}$$

Интегрируем:

$$c_-^{(1)}(\infty) = \int\limits_{-\infty}^{\infty} d\theta \cdot e^{-i\int_0^t \omega_{+-}(\tau)d\tau} \frac{\langle\psi_-(\theta)|\frac{\partial\hat{H}}{\partial\theta}|\psi_+(\theta)\rangle}{2\gamma\operatorname{ch}\theta},$$

where

$$\langle\psi_-(\theta)|\frac{\partial\hat{H}}{\partial\theta}|\psi_+(\theta)\rangle = \frac{1}{2\operatorname{ch}\theta}\begin{pmatrix} e^{-\theta/2} & -e^{\theta/2} \end{pmatrix}\begin{pmatrix} \gamma\operatorname{ch}\theta & 0 \\ 0 & -\gamma\operatorname{ch}\theta \end{pmatrix}\begin{pmatrix} e^{\theta/2} \\ e^{-\theta/2} \end{pmatrix} = \gamma,$$

$$\int\limits_0^t \omega_{+-}(\tau)d\tau = 2\frac{\gamma^2}{\alpha}\int\limits_0^\theta \operatorname{ch}^2\theta d\theta = \frac{\gamma^2}{\alpha}\left[\theta + \frac{1}{2}\operatorname{sh}2\theta\right].$$

And we get the final formula:

$$c_-^{(1)}(\infty) = \int\limits_{-\infty}^{\infty} \frac{\exp\left(-i\frac{\gamma^2}{\alpha}\left(\theta + \frac{1}{2}\operatorname{sh}2\theta\right)\right)}{2\operatorname{ch}\theta}d\theta$$

Now, it is relatively easy to proceed. We have a an integral of the form "fast-oscillating function + slow envelope". Integrals of this type are taken by the stationary phase method, or more generally by the pass method. Here, the phase $f(\theta) = \theta + \frac{1}{2}\operatorname{sh}2\theta$, which has $f'(\theta) = 1 + \operatorname{ch}2\theta \geq 2$, поэтому точек стационарной фазы на вещественной оси нет. (?????????????) Для этого мы можем сделать так, чтобы в экспоненте стояла линейная функция, перейдя к интегралу по $z = \theta + \frac{1}{2}\operatorname{sh}2\theta \to dz = d\theta(1 + \cos 2\theta) = 2\operatorname{ch}^2\theta d\theta$, и переписав интеграл в виде:

$$c_-^{(1)}(\infty) = \int\limits_{-\infty}^{\infty} \frac{\exp\left(-i\frac{\gamma^2}{\alpha}z\right)}{4\operatorname{ch}^3\theta}dz$$

Теперь мы можем применить лемму Жордана, замкнув контур интегрирования в нижней полуплоскости (где экспонента затухает), и сведя его к вычетам в полюсах, которые определяются из $\operatorname{ch}\theta = 0$, то есть $\theta_k = -i\frac{\pi}{2}(1+2k) = z_k$. Беря только полюс с $k = 0$, и оставляя только экспоненту, получаем:

$$c_-^{(1)}(\infty) \sim e^{-\pi\gamma^2/2\alpha}$$

В итоге

$$P \sim e^{-\pi\gamma^2/\alpha}$$

ПТФ-6.пр.1 Landau-Zener problem by adiabatics

Suppose we have a two-level system, where level spacing is changed in time and models by a Hamiltonian

$$\hat{H}(t) = \begin{pmatrix} \alpha t & \gamma \\ \gamma & -\alpha t \end{pmatrix}.$$

Here α and γ are constants.

Find a probability of transfer to the upper state at $t \to \infty$ from the lower one, on which a particle was initially (in time $t \to -\infty$).

Solution

(the solution is exactly the same, as it was for the transfer vice versa. The answer is the same. But it is a good practice, to do carefully all transformations again, assuming that initial state is purely different.)

(??? by the way, why do we expect that always the probability of transfer to one direction is the same for transfer to another? Which exactly part of the theory assures us about it?)

ПТФ-6.пр.2.4 Adiabatic quantum transport

Представим себе длинную двумерную полосу, ширина которой a(x) как-то медленно зависит от координаты x.

Такая задача имеет важные применения — буквально такие системы умеют создавать экспериментаторы, занимающиеся наноинженерией (см. схему).

Solution

This is the basic example for stationary adiabatics methods.

Если бы ширина не изменялась, то то иеременшые разделялись бы, и точное решение гамильтониаша иредставлялось бы в виде $\psi_{p,n}(x,y) = e^{ipx}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi n y}{a} - \frac{\pi n}{2}\right)$ (если стешка соответствует $y \in \left(-\frac{a}{2}; \frac{a}{2}\right)$; эиергия такого состояния равнялась бы $E_{p,n} = \frac{p^2}{2m} + \frac{\pi^2 n^2}{2ma^2}$. Когда ширина как-то неявно зависит от координаты x, то мы можем иримснить адиабати-

мы в первую очередь должны зафиксировать координату x и решить задачу для быстрой подсистемы.

Решение записывается тривиально: $\psi_n^{(f)}(y,x) = \sqrt{\frac{2}{a(x)}}\sin\left[\frac{\pi n y}{a(x)} - \frac{\pi n}{2}\right], E_n^{(f)}(x) = \frac{\pi^2 n^2}{2ma^2(x)}$. В результате для оставшегося эффективного одномерного движения мы можем записать эффективный гамильтониан:

$$\hat{H}_{eff} = \frac{\hat{p}_x^2}{2m} + \frac{\pi^2 n^2}{2ma^2(x)}$$

Дальше можно уже работать с этим гамильтонианом - к примеру, интересна задача рассеяния, когда электрон запускают с фиксированной энергией E с $x \to -\infty$, и интересуются, с какой вероятностью он пройдёт через такое сужение.

Однако решение оставшейся одномерной задачи (скажем, когда $a(x)$ задано явно) уже производится другими методами, которые обсуждаются в других семинарах, поэтому на этом мы остановимся.

В данной задаче адиабатическое приближение, как всегда, будет работать, покуда не будут возбуждаться другие поперечные моды.

Это будет верно, если потенциал плавный и не может передать частице импульс порядка $\delta p \sim \frac{1}{a}$ – а значит, масштаб типичного изменения величины $a(x)$ должен быть меньше самой величины $a(x)$: $\frac{da}{dx} \ll 1$.

ПТФ-6.пр.2.5 Particle in ellipse

Let the free particle be placed in a strongly elongated ellipse $\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1, a \gg b$. Find low-lying energy levels.

Note that there is a well-known solution for a circle (when $a = b$), and there is also a solution for the slightly deformed circle (when $\frac{|a-b|}{a} \ll 1$) by perturbation theory.

Solution

This is the basic example for stationary adiabatic methods.

Типичный энергетический масштаб поперечного движения (вдоль y) - это $\omega^{(f)} \sim \frac{1}{mb^2}$, большая величина; из этого мы заключаем, что нонеречное движение - быстрое, а продольное - медленное.

We write the effective Hamiltonian for the motion along x axes (отличие в том, что теперь $y \in (-y(x), y(x))$) from

$$\psi_n^{(f)}(y,x) = \frac{1}{\sqrt{y(x)}} \sin\left[\frac{\pi n y}{2y(x)} - \frac{\pi n}{2}\right] \qquad E_n^{(f)} = \frac{\pi^2 n^2}{8my^2(x)}$$

as

$$\hat{H}_{\text{eff}} = \frac{\hat{p}_x^2}{2m} + \frac{\pi^2 n^2}{8my^2(x)} = \frac{\hat{p}_x^2}{2m} + \frac{\pi^2 n^2}{8mb^2}\left(1 - \frac{x^2}{a^2}\right)^{-1} \overset{x \ll a}{\approx} \frac{\hat{p}_x^2}{2m} + \frac{\pi^2 n^2}{8mb^2}\left(1 + \frac{x^2}{a^2}\right)$$

This potential corresponds to the oscillator with $\omega_N = \frac{\pi N}{2mab}$. Из этого мы заключаем, что уровни энергии можно приближённо записать как:

$$E_{N,n} = \frac{\pi^2 N^2}{8mb^2} + \frac{\pi N}{2mab}\left(n + \frac{1}{2}\right)$$

(????? I should learn better theory, why it is so???)

Отметим, что типичное расстояние между «быстрыми» подуровнями оценивается как $\Delta E^{(f)} \sim \frac{1}{mb^2}$, а между «медленными» - как $\Delta E^{(s)} = \omega \sim \frac{1}{mab}$, и несложно видеть, что $\Delta E^{(f)} \gg \Delta E^{(s)}$, поэтому адиабатическое приближение оправдано. В этом смысле, для буквально низколежащих уровней энергии необходимо положить $N = 1$.

Второе, что необходимо проверить - что разложение по x/a тоже было законным. Движение вдоль оси x в нашем решении соответствует осциллятору, у которого масштаб волновой функции - это $x_0 \sim \frac{1}{\sqrt{m\omega}} = \sqrt{ab} \ll a$ - поэтому это приближение тоже работает.

Relation to chaos (???)

Наконец, отметим, что такую же задачу можно было бы поставить и в классической механике, в которой частицу с фиксированным импульсом запускают в такой эллиптический бильярд. В таком случае уже с классической точки зрения, поперечное движение было бы быстрым (это означает, что прежде чем x-компонента импульса поменяет знак, произойдёт огромное количество столкновений вдоль оси y), а вдоль оси x частица бы испытывала практически гармонические колебания.

(??? I don't know relation to chaos, here there is no chaos, there there is chaos....)

ПТФ-6.пр.2.6 Частица в конусе

(выпишу потом эту задачу из их конспектов)

Б-2.8.14 Фаза берри мюона в магнитном поле (??)

Рассмотреть задачу о покоящемся положительном мюоне, находящемся в однородном магнитном поле. Напряженность поля $\mathcal{H}$ составляет постоянный угол θ с осью z и медленно вращается вокруг нее. Предполагая, что вектор $\mathcal{H}$ совершает полный оборот вокруг оси z, определить фазу Берри.

Reminder: the Berry's phase is $\gamma := \int\limits_0^T dt\dot{\gamma}(t) = i \oint_\Gamma d\xi \langle\psi_n(\xi(t))|\frac{\partial}{\partial\xi}|\psi_n(\xi(t))\rangle$ and muon is just spin 1/2 particle.

Solution.

Состояния с определенными значениями проекции спина $S_{\mathcal{H}} = \pm 1/2$ на направление магнитного поля определяются векторами (см. задачу 2.4.19)

$$|+\rangle_{\mathcal{K}} = \cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}e^{i\varphi}|-\rangle,$$
$$|-\rangle_{\mathcal{K}} = -\sin\frac{\theta}{2}|+\rangle + \cos\frac{\theta}{2}e^{i\varphi}|-\rangle,$$

где векторы $|+\rangle$ и $|-\rangle$ описывают состояния с положительной и отрицательной проекциями спина на ось z (см. (II.26)).

Два состояния $|\pm\rangle_{\mathcal{K}}$ (1) отвечают значениям энергии $\mp\mu_0\mathcal{H}/2$. Таким образом, энергетический спектр невырожден. Пусть теперь магнитное поле адиабатически медленно вращается вокруг оси z при постоянном угле θ (рис. 2.10). В этом случае применимо адиабатическое приближение, из которого следует, что частица, находившаяся первоначально в основном состоянии, в нем и останется, а вектор состояния будет отличаться от исходного вектора (1) фазовым множителем (найденным в формуле (2) задачи 2.8.13).

Периоду T изменения параметров соответствует изменение азимутального угла φ от 0 до 2π, поэтому для фазы Берри имеем

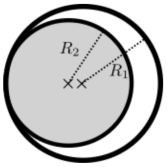
$$\gamma = i\int\limits_0^{2\pi} d\varphi\mathcal{H}\langle\chi|\frac{\partial}{\partial\varphi}|\chi\rangle_{\mathcal{H}} = -\frac{1}{2}\int\limits_0^{2\pi} d\varphi(1-\cos\theta) = -s\mathcal{H}\int\limits_0^{2\pi} d\varphi\int\limits_0^{\theta}\sin\theta' d\theta' = -\,\mathrm{sH}\,\Omega,$$

где Ω - телесный угол, под которым из начала координат видна траектория, описываемая средним значением спина (рис. 2.10), $s_H = 1/2$ - проекция спина на направление магнитного поля.

17.1.8 Problems about adiabatics 3: Specific Models

ПТФ-10.з1. Particle inside two cylinders

A particle of mass m is located between two infinite cylinders $|R_1 - R_2| \ll R_{1,2}$, which touch each other internally.



Find the low-lying energy levels of such a system.

Solution.

Адиабатическое разделение переменных:

$$\hat{H}(r,\varphi) = \hat{H}_s(\varphi) + \hat{H}_f(r,\varphi)$$

$$\hat{H}_s(\varphi) = -\frac{\hbar^2}{2mR_2^2}\left(\frac{\partial}{\partial\varphi}\right)^2, \quad \hat{H}_f(r,\varphi) = -\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial r}\right)^2$$

Зафиксируем положение медленной подсистемы и решим задачу для быстрой. В первом приближении пренебрегаем производной по φ:

$$\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial r}\right)^2\psi(r,\varphi) = \varepsilon^{(f)}(\varphi)\psi(r,\varphi)$$

Обозначим $k(\varphi) = \frac{2m\varepsilon^{(f)}(\varphi)}{\hbar^2}$. Тогда решение с учетом граничного условия при $r = R_2$:

$$\psi(r,\varphi) = A(\varphi)\sin(k(\varphi)(r-R_2))$$

Пусть $h(\varphi)$ – длина отрезка луча в полости между цилиндрами, идушего под углом φ (φ отсчитываем от плоскости симметрии системы), а $\Delta = R_1 - R_2$. Используя $|R_1 - R_2| \ll R_{1,2}$ и теорему косинусов, получим: (write it better and add picture!!!)

$$h(\varphi) = (R_1 - R_2)(1+\cos\varphi)$$

Граничное условия на внешнем цилиндре:

$$\psi(R_2 + h(\varphi),\varphi) = 0 \to k_N(\varphi) = \frac{\pi N}{(1+\cos\varphi)\Delta}$$

Соответствующие нормированные волновые функции:

$$\psi_N^{(f)} = \sqrt{\frac{2}{\Delta(1+\cos\varphi)}}\sin\left(\frac{\pi N(r-R_2)}{(1+\cos\varphi)\Delta}\right)$$

Уровни энергии быстрой подсистемы:

$$\varepsilon_N(\varphi) = \frac{\hbar^2\pi^2N^2}{2m\Delta^2(1+\cos\varphi)^2}$$

$$-\frac{\hbar^2}{2mR_2^2}\frac{d^2\psi_N(\varphi)}{d\varphi^2} + \frac{\hbar^2\pi^2N^2}{2m\Delta^2(1+\cos\varphi)^2}\psi_N(\varphi) = E_N^{(s)}\psi_N(\varphi)$$

Сведём задачу к гармоническому осциллятору. Разложим по малому углу φ:

$$-\frac{\hbar^2}{2mR_2^2}\frac{d^2\psi_N(\varphi)}{d\varphi^2} + \frac{\hbar^2\pi^2N^2}{2m\Delta^2(1+\cos\varphi)^2}\psi_N(\varphi) = E_N^{(s)}\psi_N(\varphi)$$

Уровни энергии:

$$E_{N,n} = \frac{\hbar^2\pi^2N^2}{8m(R_1-R_2)^2} + \frac{\hbar^2\pi N}{2\sqrt{2}mR_1(R_1-R_2)}\left(n+\frac{1}{2}\right)$$

ПТФ-10.з.2. Поправки к энергии в эллипсе (???)

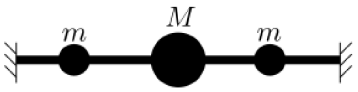
Определите ведущую поправку к энергии основного состояния свободной частицы в эллиптической полости с полуосями $a \gg b$.

Solution.

(на семинаре по идее она разобрана, пропишу потом.)

ПТФ-10.з3. Three big particles in a box

В одномерный ящик ширины L помещены три частицы, две из которых имеют массу m, а третья находится между ними и имеет массу $M \gg m$. Частицы взаимодействуют точечным образом так, что они оказываются непроницаемы друг для друга. Определите низколежащие уровни энергии такой системы.



Solution.

Гамильтониан системы:

$$\hat{H} = -\frac{1}{2m}\left(\frac{\partial}{\partial x_1}\right)^2 - \frac{1}{2m}\left(\frac{\partial}{\partial x_2}\right)^2 - \frac{1}{2M}\left(\frac{\partial}{\partial X}\right)^2 + U(x_1,x_2,X)$$

где $x_{1,2}$ – координаты частиц m, X – координата частицы M. $U(x_1,x_2,X) = U_1(x_1,X) + U_2(x_2,X)$ – потенциальная энергия взаимодействия частиц, обеспечивающая непроницаемость. Частица M – медленная подсистема, а частицы m в совокупности – быстрая.
Адиабатическое приближение:

$$\hat{H}_f = -\frac{1}{2m}\left(\frac{\partial}{\partial x_1}\right)^2 - \frac{1}{2m}\left(\frac{\partial}{\partial x_2}\right)^2 + U_1(x_1,X) + U_2(x_2,X), \quad \hat{H}_s = -\frac{1}{2M}\left(\frac{\partial}{\partial X}\right)^2$$

Волновые функции шариков m, соответствующие $\hat{H}_f$:

$$\psi_{1,N_1}(x_1,X) = \sqrt{\frac{2}{X}}\sin\left(\frac{\pi N_1}{X}x_1\right), \quad \psi_{2,N_2}(x_2,X) = \sqrt{\frac{2}{L-X}}\sin\left(\frac{\pi N_2}{L-X}(L-x_2)\right)$$

$$\psi_{N_1,N_2}(x_1,x_2,y)=\frac{2}{\sqrt{y(L-y)}}\sin\left(\frac{\pi N_1}{y}x_1\right)\cdot\sin\left(\frac{\pi N_2}{L-y}(L-x_2)\right)$$

Энергия – сумма энергий каждого движения:

$$\varepsilon^{(f)}_{N_1,N_2}=\frac{\pi^2}{2m}\left(\frac{N_1^2}{X^2}+\frac{N_2^2}{(L-X)^2}\right)$$

Эффективная потенциальная энергия для медленной подсистемы:

$$\hat{H}^{(\text{eff})}_s(X)=\frac{\hat{p}_X^2}{2M}+\frac{\pi^2}{2m}\left(\frac{N_1^2}{X^2}+\frac{N_2^2}{(L-X)^2}\right)$$

Минимум энергии находится в точке: $X_0=\frac{L}{1+(N_2/N_1)^{2/3}}$.

$$U''_{\text{eff}}(X_0)=\frac{3\pi^2}{mL^4}\left(N_1^2\left(1+\left(\frac{N_2}{N_1}\right)^{2/3}\right)^4+N_2^2\left(1+\left(\frac{N_1}{N_2}\right)^{2/3}\right)^4\right)$$

$$E_{N_1,N_2,n}=\frac{\pi^2}{2mL^2}\left(N_1^2\left(1+\left(\frac{N_2}{N_1}\right)^{2/3}\right)^2+N_2^2\left(1+\left(\frac{N_1}{N_2}\right)^{2/3}\right)^2\right)+$$
$$+\sqrt{\frac{3\pi^2}{MmL^4}\left(N_1^2\left(1+\left(\frac{N_2}{N_1}\right)^{2/3}\right)^4+N_2^2\left(1+\left(\frac{N_1}{N_2}\right)^{2/3}\right)^4\right)}\left(n+\frac{1}{2}\right)$$

Я. Частица в треугольнике (!?!?)

(?? а тут то что делать??)

ПТФ-10.з4. Particle in a ring with strong magnetic field

A particle with spin $1/2$ of mass m moves along a ring of radius R. A magnetic monopole is placed in the center of the ring, which creates a large magnetic field B on the ring. The Hamiltonian of such a system has the form:

$$\hat{H}=-\frac{1}{2mR^2}\partial_\varphi^2-\mu_B B(\cos\varphi\hat{\sigma}_x+\sin\varphi\hat{\sigma}_y)$$

Determine the energy levels of such a system in the limit $\mu_B B\gg\frac{1}{mR^2}$.

Solution.

$$\hat{H}=-\frac{1}{2mR^2}\left(\frac{d}{d\varphi}\right)^2-\mu_0 B\begin{pmatrix}0 & e^{-i\varphi}\\ e^{i\varphi} & 0\end{pmatrix}$$

Медленная подсистема – движение по углу, быстрая – вращение спина:

$$\hat{H}=\hat{H}_s+\hat{H}_f,\quad \hat{H}_s=-\frac{1}{2mR^2}\left(\frac{d}{d\varphi}\right)^2,\quad \hat{H}_f=-\mu_0 B\begin{pmatrix}0 & e^{-i\varphi}\\ e^{i\varphi} & 0\end{pmatrix}$$

Зафиксируем положение медленной подсистемы и решим стационарное уравнение Шрёдингера для быстрой:

$$\hat{H}_f|\psi^{(f)}\rangle=\varepsilon^{(f)}|\psi^{(f)}\rangle$$
$$\varepsilon^{(f)}_-=-\mu_0 B_0,\quad \varepsilon^{(f)}_+=+\mu_0 B_0$$
$$|\psi^{(f)}_-\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}-e^{-i\varphi}\\ 1\end{pmatrix},\quad |\psi^{(f)}_+\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}e^{-i\varphi}\\ 1\end{pmatrix}$$

Представим полную волновую функцию в виде:

$$|\psi(\varphi)\rangle\equiv f_+(\varphi)|\psi^{(f)}_+\rangle+f_-(\varphi)|\psi^{(f)}_-\rangle$$

$$\frac{d^2|\psi(\varphi)\rangle}{d\varphi^2} = f_+''(\varphi)|\psi_+^{(f)}(\varphi)\rangle + 2f_+'(\varphi)|\psi_+^{(f)}(\varphi)\rangle' + f_+(\varphi)|\psi_+^{(f)}(\varphi)\rangle''+$$
$$+ f_-''(\varphi)|\psi_-^{(f)}(\varphi)\rangle + 2f_-'(\varphi)|\psi_-^{(f)}(\varphi)\rangle' + f_-(\varphi)|\psi_-^{(f)}(\varphi)\rangle''$$

Подставим в гамильтониан и получим систему уравнений на $f_\pm(\varphi)$:

(??? это непонятно, как оно получается?? I remember that I thought about it, but still, currently I should think again about it)

$$\begin{cases} f_+''(\varphi) + if_+'(\varphi) - \frac{1}{2}f_+(\varphi) - if_-'(\varphi)e^{-2i\varphi} - \frac{f_-(\varphi)}{2}e^{-2i\varphi} + 2mR^2\mu_0 B f_+(\varphi) = -2mR^2 E f_+(\varphi) \\ f_-''(\varphi) - if_-'(\varphi) - \frac{1}{2}f_-(\varphi) + if_-'(\varphi)e^{2i\varphi} - \frac{f_+(\varphi)}{2}e^{2i\varphi} - 2mR^2\mu_0 B f_-(\varphi) = -2mR^2 E f_-(\varphi) \end{cases}$$

Ищем решение в виде:

$$f_\pm(\varphi) = \alpha_\pm e^{i\omega_\pm \varphi}$$

Граничные условия:

$$\begin{cases} |\psi(0)\rangle = |\psi(2\pi)\rangle \\ |\psi(0)\rangle' = |\psi(2\pi)\rangle' \end{cases}$$

$$\begin{cases} f_\pm(0) = f_\pm(2\pi) \\ f_\pm'(0) = f_\pm'(2\pi) \end{cases} \quad \to \omega_\pm = n_\pm \in \mathbb{Z}$$

$$\begin{cases} \alpha_+\left(n_+^2 - n_+ - \frac{1}{2} + 2mR^2\mu_0 B + 2mR^2 E\right) + \alpha_-\left(n_- - \frac{1}{2}\right) = 0 \\ \alpha_-\left(n_-^2 + n_- - \frac{1}{2} - 2mR^2\mu_0 B + 2mR^2 E\right) - \alpha_+\left(n_+ + \frac{1}{2}\right) = 0 \end{cases}$$

$$\left((n+2)^2 - n - \frac{5}{2} + 2mR^2\mu_0 B + 2mR^2 E\right)\left(n^2 + n - \frac{1}{2} - 2mR^2\mu_0 B + 2mR^2 E\right) = -\left(n - \frac{1}{2}\right)\left(n + \frac{5}{2}\right)$$

Для $2mR^2\mu_0 B \gg 1$, $n \ll \sqrt{2mR^2\mu_0 B}$:

$$\left(2mR^2\mu_0 B + 2mR^2 E\right)\left(-2mR^2\mu_0 B + 2mR^2 E\right) \approx -\left(n - \frac{1}{2}\right)\left(n + \frac{5}{2}\right)$$

$$E^2 \approx \mu_0^2 B^2 - \frac{\left(n - \frac{1}{2}\right)\left(n + \frac{5}{2}\right)}{4m^2R^4}$$

$$E_n \approx \pm\mu_0 B \mp \frac{\left(n - \frac{1}{2}\right)\left(n + \frac{5}{2}\right)}{8m^2R^4\mu_0 B}$$

(add from English)Г-8.59.

Гамильтониан системы имеет вид

$$\hat{H} = \frac{1}{2m}\hat{p}_x^2 + \frac{1}{2M}\hat{p}_y^2 + \frac{k\left(x^2 + y^2\right)}{2} + \alpha xy, \quad |\alpha| < k,$$

причем $M \gg m$ (два связанных осциллятора с сильно различающимися массами). Найти уровни энергии системы и соответствующие им волновые функции на основе адиабатического приближения. Сравнить полученный результат с точным решением, см. 2.50.

(add from English)Г-8.60.

Две частицы с сильно различающимися массами $M \gg m$ находятся в бесконечно глубокой потенциальной яме ширины и взаимодействуют друг с другом как взаимно непроницаемые точки. Найти энергетические уровни нижней части спектра и соответствующие им волновые функции.

(add from English)Г-8.61.

Используя адиабатическое приближение, обсудить вопрос об энергетическом спектре и виде соответствующих волновых функций связанных состояний частицы в центральном потенциале притяжения $U(r)$ в присутствии достаточно сильного однородного магнитного поля.

Найти сдвиги уровней Ландау под влиянием короткодействующего потенциала, а также основной уровень атома водорода в сильном магнитном поле.

TM. Ionization with moving δ-potential

A 1D particle is located in the δ-potential. It starts moving slowly by a hyperbolic tangents law. Find a probability of ionization.
(add a plot of a hyperbolic tangent)

Solution

(use that formula from adiabatics, but I need to practice more in it)

Feigelman.EntrExam.th-4/8

Particle with strongly anisotropic spectrum $E = \frac{p_x^2}{2m_1} + \frac{p_x^2+p_y^2}{m_2}$, $m_1 \gg m_2$, is moving in the attractive potential $U(r) = -\alpha/r$. Find few low-lying energy levels.

Solution by Oleg Baburin.

(??? write here why we do so!!!)

1. Разделим переменные:

$$\Psi(\rho, z) = R_{00}(\rho)\chi(z)$$

2. В атомных единицах:

$$\hat{\boldsymbol{p}}_\perp = -i\boldsymbol{\nabla}_\perp \quad \Rightarrow \quad \hat{p}_\perp^2 = -\Delta_\perp$$

3. Поперечное состояние:

$$R_{00}(\rho) = 4e^{-2\rho}$$

4. Дифференцируем:

$$\frac{dR_{00}}{d\rho} = -8e^{-2\rho}, \quad \frac{d^2R_{00}}{d\rho^2} = 16e^{-2\rho}$$

Теперь подействуем оператором $\hat{p}_\perp^2$ на $R_{00}(\rho)$:

$$\frac{\hat{p}_\perp^2}{2}R_{00}(\rho) = \left(\frac{1}{\rho} - 2\right)R_{00}(\rho)$$

(!!! write here the approximation that is done. it is a cool approximation, we integrate over R00 also!!)
5. Получаем эффективный одномерный гамильтониан:

$$\left[\frac{\hat{P}_z^2}{2m_1} - \left\langle \frac{1}{\sqrt{\rho^2+\varepsilon^2 z^2}} - \frac{1}{\rho} \right\rangle\right]\chi(z) = (E+2)\chi(z)$$

6. Интеграл:

$$\left\langle \frac{1}{\rho} - \frac{1}{\sqrt{\rho^2+\varepsilon^2 z^2}} \right\rangle = 16J(a), \quad a := \varepsilon|z|$$

Где:

$$J(a) = \int_0^\infty e^{-4\rho}\left[1 - \frac{\rho}{\sqrt{\rho^2+a^2}}\right]d\rho$$

Для малых a :

$$J(a) = a + O\left(a^2\right), \quad (a \to 0)$$

Подставляем:

$$\left\langle \frac{1}{\rho} - \frac{1}{\sqrt{\rho^2 + \varepsilon^2 z^2}} \right\rangle = 16\varepsilon|z| + O\left(\varepsilon^2 z^2\right)$$

7. Сведение к уравнению Эйри Подставляем полученный эффективный потенциал в одномерное уравнение:

$$-\frac{\hbar^2}{2m_1}\chi''(z) - F|z|\chi(z) = \mathcal{E}\chi(z)$$

где $\mathcal{E} = E + 2$. Для $z > 0$:

$$\chi''(z) + \frac{2m_1 F}{\hbar^2}\left(z + \frac{\mathcal{E}}{F}\right)\chi(z) = 0$$

Вводим характеристическую длину:

$$\ell = \left(\frac{\hbar^2}{2m_1 F}\right)^{1/3}$$

и безразмерную переменную:

$$u = \frac{z}{\ell} + \frac{\mathcal{E}}{F\ell}.$$

Получаем уравнение Эйри:

$$\frac{d^2\chi}{du^2} + u\chi = 0$$

Решение для $z \to +\infty$:

$$\chi(z) = C\mathscr{A}i(u),$$

где $\mathscr{A}i(u)$ - это функция Эйри. Из чётности потенциала $-F|z|$ получаем условия на $z = 0$:

$$\text{нечётные: } \chi(0) = 0 \Rightarrow \mathscr{A}i\left(\frac{\mathcal{E}}{F\ell}\right) = 0,$$
$$\text{чётные: } \chi'(0) = 0 \Rightarrow \mathscr{A}i'\left(\frac{\mathcal{E}}{F\ell}\right) = 0.$$

8. Уровни энергии Обозначим нули функции Эйри как β_n для нечётных состояний и δ_n для чётных состояний. Тогда уровни энергии для эффективной одномерной задачи будут:

$$\mathcal{E}_n = \left(\frac{F^2\hbar^2}{2m_1}\right)^{\frac{1}{3}} \begin{cases} \beta_n, & \text{нечётные} \\ \delta_n, & \text{чётные} \end{cases}$$

9. Итоговая формула для энергии Подставляем $F = 16\alpha\varepsilon$. Итого:

$$\text{для нечетных: } \mathrm{E}_n = \alpha^2 m_1\left(-2 + 2^{\frac{7}{3}}\varepsilon^{\frac{2}{3}}\beta_n\right) \text{ для четных: } \mathrm{E}_n = \alpha^2 m_1\left(-2 + 2^{\frac{7}{3}}\varepsilon^{\frac{2}{3}}\delta_n\right)$$

17.1.9 Simple Problems about adiabatics in Condensed Matter

El-Batanouny.10.1 Dirac and Berry

Consider Dirac fermions in two dimensions described by the Hamiltonian

$$\mathcal{H}(\mathbf{k}) = \sum_{\alpha} d_{\alpha}(\mathbf{k})\sigma_{\alpha}, \quad d_1(\mathbf{k}) = k_x, d_2(\mathbf{k}) = k_y, d_3(\mathbf{k}) = m.$$

(a) Show that the Berry connection of the lower band can be written as

$$\mathcal{A}_{\mu} = i\langle\psi_{-}(\mathbf{k})|\partial_{k_\mu}\psi_{-}(\mathbf{k})\rangle = -\frac{1}{2d(\mathbf{k})\left[d(\mathbf{k}) - d_3(\mathbf{k})\right]}\left[d_2(\mathbf{k})\partial_{k_\mu}d_1(\mathbf{k}) - d_1(\mathbf{k})\partial_{k_\mu}d_2(\mathbf{k})\right]$$

where $d(\mathbf{k}) = |\mathbf{d}(\mathbf{k})|$.
(b) Show that the corresponding Berry curvature is given by

$$\mathcal{F}_{\mu\nu}(\mathbf{k}) = \frac{1}{2}\epsilon_{\alpha\beta\gamma}\hat{d}_{\alpha}\partial_{k_\mu}\hat{d}_{\beta}\partial_{k_\nu}\hat{d}_{\gamma}, \quad \hat{\mathbf{d}}(\mathbf{k}) = \frac{\mathbf{d}(\mathbf{k})}{|\mathbf{d}(\mathbf{k})|}.$$

Solution.

(??? I think it is nearly fully useless problem, so I'll think about it very later)
(!!! вспомню автора книги - переназову задачу!!!)

El-Batanouny.10.2 Parallel transport gauge

Consider a system subject to a weak adiabatic perturbation that is periodic in time. With the total Hamiltonian $\mathcal{H}(t+T) = \mathcal{H}(t)$, a general state $|\psi(t)\rangle$ obeys the Schrödinger equation

$$i\partial_t|\psi(t)\rangle = \mathcal{H}(t)|\psi(t)\rangle$$

and can be expressed as

$$|\psi(t)\rangle = \sum_{\ell'} \exp\left[-\frac{i}{\hbar}\int_0^t dt'\varepsilon_{\ell'}(t')\right] c_{\ell'}(t)|\ell'(t)\rangle,$$

where $|\ell'(t)\rangle$ is an eigenket of $\mathcal{H}(t)$, which are single-valued in $t : |\ell'(t+T)\rangle = |\ell'(t)\rangle$.
(a) Use the Schrödinger equation to derive an expression for $\dot{c}_{\ell}(t)$.
(b) Parallel transport, or horizontal lift, requires that

$$\langle\tilde{\ell}(t)|\partial_t\tilde{\ell}(t)\rangle \equiv \langle\bar{\ell}(\eta)|\mathrm{d}|\tilde{\ell}(t\eta)\rangle\frac{d\eta}{dt} = 0.$$

Show that the horizontal lift condition is satisfied by the gauge transformation

$$|\ell(t)\rangle \to |\bar{\ell}(t)\rangle = \exp\left[i\int_0^t dt'|\ell(t')\,|\partial_{t'}\ell(t')\rangle\right]|\ell(t)\rangle$$

(c) If the system starts in the eigenstate $|\tilde{\ell}(0)\rangle$, so that $c_{\ell} = 1, c_{\ell} = 0, \ell' \neq \ell$.
(i) Determine $\dot{c}_{\ell}$ and $\dot{c}_{\ell}$. Is the adiabatic theorem satisfied?
(ii) Check if the ansatz solution

$$c_{\ell'}(t) = -i\hbar\frac{\langle\bar{\ell}'(t)|\partial_t\bar{\ell}(t)\rangle}{\varepsilon_{\ell}(t) - \varepsilon_{\ell'}(t)}\exp\left[-\frac{i}{\hbar}\int_0^t dt'\left(\varepsilon_{\ell}(t') - \varepsilon_{\ell'}(t')\right)\right]$$

obeys the differential equation you obtained for $\dot{c}_{\ell}$. (Neglect terms of 2nd order).
(iii) Write down an expression for the state function that includes the first-order approximation.

Solution.

El-Batanouny.10.3 Divergence of Berry curvature

Use expression (10.24) to show that for $E_m \neq E_n$,

$$\nabla \cdot \mathcal{F} = 0.$$

Hint: Use the Hermitian operator

$$\mathbf{O} = -i \sum_n |\nabla n\rangle\langle n|$$

to express (10.24) as

$$\mathcal{F} = \mathrm{Im}\langle n|\mathbf{O} \times \mathbf{O}|n\rangle.$$

Solution.

El-Batanouny.10.4

In Section 10.3, we derived Berry's curvature for the two-level system using two methods: the direct geometric method, and the one- and two-form method. Alternatively, use the Hamiltonian derivative method outlined in Section 2.2.3 to derive Berry's curvature for that system.

Solution.

El-Batanouny.10.5

Consider a spin-J particle in a slowly rotating magnetic field. The Hamiltonian is given by

$$\mathcal{H} = -\boldsymbol{\mu} \cdot \mathbf{J}$$

where $\mathbf{J}$ is the spin angular momentum operator, and $\boldsymbol{\mu} = \mu_B \mathbf{B}(\hat{\mathbf{n}}(t))$. Use the Hamiltonian derivative method of Section 2.2.3 to determine the state Berry curvature and the corresponding Berry phase.

Solution.

El-Batanouny.10.6

We shall consider the ABE ring of Section 10.3 from a different perspective. We shall look at the system as consisting of a one-dimensional metallic ring with circumference L, threaded by a magnetic flux Φ. The Hamiltonian is again

$$\mathcal{H} = \frac{1}{2m_e}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2, \quad \nabla \times \mathcal{A} = 0.$$

We may recast the ring into a one-dimensional periodic structure of period L, by defining $x = L\varphi/2\pi$.

(a) If we write $\mathcal{A} = \nabla\chi(x)$, what will $\chi(x)$ be?

(b) Perform a gauge transformation on the one-dimensional Hamiltonian to eliminate $\mathcal{A}$. What boundary conditions have to be applied to the solutions of the corresponding Schrödinger equation?

(c) Determine the eigenfunctions and energy spectrum, by writing the solution in the Bloch form Ae^{ikx} and applying the boundary conditions you obtained in part (b).

(d) Calculate the current carried by an electron in a state $n, I_n(\phi) = ev_n/L = \frac{e}{\hbar L}\frac{\partial E_n}{\partial k_n}$.

(e) Let us fill the ring with and odd number N_{odd} of electrons, at zero temperature. What is the total current flowing through the system, $I(\phi)$? What happens when $\phi = \phi_0/2$?

(f) How does the current change when the number of electrons in the ring is even?

Solution.

El-Batanouny.10.7 Spin-orbit coupling in an ABE-like configuration

An electron is constrained to move on a 1D ring of radius a. The electron experiences a spin-orbit interaction with the electric field created by a charge Q placed at the center of the ring.

1. Write the Hamiltonian $\mathcal{H}(x, p, \mathbf{s})$.

2. Determine the electron eigenenergies and corresponding velocities.

3. Determine that the magnetic flux Φ through the ring would cancel the interaction of Q with a spin up electron.

Solution.

El-Batanouny.10.8

We consider the case of a time-reversal symmetric system with half-integer spin, represented by a Hamiltonian $\mathcal{H}(\eta)$, with $\eta = [\eta_1, ..., \eta_n]$. We label degenerate orthonormal Kramers' pair eigenkets as $|\mu, \eta\rangle, \mu = \pm 1$, that are smooth functions of the parameters η within a given patch. We need to define a new Berry connection A_ℓ, which is a 2×2 matrix, as

$$A_\ell^{\mu v}(\eta) = i\langle \mu, \eta | \partial_\ell | v, \eta \rangle,$$

where ∂_ℓ is the partial derivative with respect to η_ℓ. A gauge transformation to a basis set $|\mu, \eta\rangle'$, is obtained via a unitary transformation

$$|\mu, \eta\rangle' = \sum_\nu |v, \eta\rangle U_{v\mu}(\eta),$$

where $U(\eta)$ is a 2×2 unitary matrix that varies smoothly with η .[14] The non-Abelian Berry curvatures corresponding to the Berry connections $\mathcal{A}_\ell$ are defined as

$$\mathcal{F}_{\ell\ell'} = \partial_\ell \mathcal{A}_{\ell'} - \partial_{\ell'} \mathcal{A}_\ell - i\left[\mathcal{A}_\ell, \mathcal{A}_{\ell'}\right].$$

(a) Show that If $\boldsymbol{\Theta}|+, \boldsymbol{\eta}\rangle = |-, \boldsymbol{\eta}\rangle e^{i\phi} \rightarrow \boldsymbol{\Theta}|-, \boldsymbol{\eta}\rangle = -|+, \boldsymbol{\eta}\rangle e^{i\phi}$.

(b) Derive an expression for the Berry connection $\overline{\mathcal{A}}_\ell$, corresponding to the new states $|\mu, \eta\rangle'$, in terms of $\mathcal{A}_\ell$ and $U(\eta)$.

(c) Derive an expression for the Berry curvature $\overline{\mathcal{F}}_{\ell\ell'}$

$$\overline{\mathcal{F}}_{\ell\ell'} = \partial_\ell \overline{\mathcal{A}}_{\ell'} - \partial_{\ell'} \overline{\mathcal{A}}_\ell - i\left[\overline{\mathcal{A}}_\ell, \overline{\mathcal{A}}_{\ell'}\right]$$

in terms of $\mathcal{F}_{\ell\ell}$ and $U(\eta)$.

Solution.

El-Batanouny.10.9

In our consideration of the trimer problem, we only included coupling between the electronic orbitals and the E_g vibronic states linear in Q. Here, we will include a higher-order quadratic coupling term; it takes the form

$$gQ^2\left(-\cos(2\varphi)\sigma_z - \sin(2\varphi)\sigma_x\right), \quad g \ll 1.$$

This term becomes important when Q is large, since it depends on Q^2.

(a) Add the quadratic terms to the Hamiltonian matrix in (10.32), and determine the electronic energy eigenvalues.

(b) The modified Hamiltonian can still be mapped onto the spin-1/2 system Hamiltonian. Write down the eigenkets in terms of a new phase angle θ and define θ in terms of the Hamiltonian matrix components.

(c) Express the effective ion potential in terms of the new electronic eigenenergies and determine its degeneracy points.

Solution.

17.1.10 Problems about adiabatics in Applications

(write about which experiments do really use this method?)

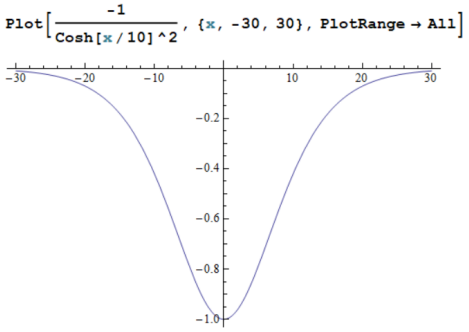
17.1.11 Problems about quasiclassical method 1: Easy Templates

ГК-1.17. Semiclassics in $V = -\frac{V_0}{\mathrm{ch}^2 \frac{x}{a}}$

For the potential $V = -\frac{V_0}{\mathrm{ch}^2 \frac{x}{a}}$, determine the energy levels and the total number of discrete levels in the quasi-classical approximation.

Solution.

This is a typical problem about WKB method. It is very easy one, except that one needs to take the integral, which can be a very big problem.



Reminder: the energy levels E_n are determined from the Bohr quantization rule

$$\int_{x_1}^{x_2} p dx = \pi \left(n + \frac{1}{2}\right) \hbar; \qquad p = \sqrt{2\mu \left(E_n + \frac{V_0}{\mathrm{ch}^2 \frac{x}{a}}\right)}$$

x_1 and x_2 are the turning points determined from the condition $p = 0$ (with $E_n < 0$ for the considered case of a discrete spectrum).

On needs to calculate the integral

$$I(E) = \int_{x_1}^{x_2} \sqrt{2\mu \left(E + \frac{V_0}{\mathrm{ch}^2 \frac{x}{a}}\right)} dx.$$

We differentiate both parts by E. In this case, the derivative of the integral along the upper and lower limits vanishes, since at points x_1 and x_2 the root expression is zero. Thus,

$$\frac{dI}{dE} = \mu \int_{x_1}^{x_2} \frac{dx}{\sqrt{2\mu \left(E + \frac{V_0}{\mathrm{ch}^2 \frac{x}{a}}\right)}}.$$

By replacing the variable $\mathrm{sh}\, \frac{x}{a} = z$, the last integral is reduced to the following form:

$$\frac{dI}{dE} = \mu a \int_{\varepsilon_1'}^{\varepsilon_3} \frac{dz}{\sqrt{2\mu \left[E\left(1 + z^2\right) + V_0\right]}} = \frac{\mu a}{\sqrt{-2\mu E}} \pi.$$

(???? I STILL HAVE NOT SOLVED THIS INTEGRAL, PLEASE HELP ME!!! I NEED TO LEARN THE MATH AGAIN)

From here we find

$$I(E) = -\sqrt{-2\mu a^2 E}\pi + C.$$

The constant C is determined from the condition that for $E = -V_0$, the integration region contracts to a point and from where

$$I\left(-V_0\right) = 0,$$

$I(E) = \sqrt{2\mu a^2}\left(\sqrt{V_0} - \sqrt{-E}\right)\pi$ Thus, in the quasi-classical approximation, energy levels are determined by the following expression:

$$E_n = -\frac{\hbar^2}{2\mu a^2}\left[\sqrt{\frac{2\mu a^2 V_0}{\hbar^2}} - \left(n + \frac{1}{2}\right)\right]^2 \quad (n = 0, 1, 2, ...).(2)$$

Number of levels $N = \frac{\sqrt{2\mu V_0}}{\hbar}a$. Note that the calculation of energy levels using the quantization rule (1) is legal if the number of levels is large, i.e.

$$\frac{2\mu a^2 V_0}{\hbar^2} \gg 1.$$

When this condition is fulfilled, the expression for energy levels (2) coincides with the exact formula for E_n obtained in problem 11, §1.

(???? додумаю ответ, пока не очень понял.)

By the way, one can compute the integral by residue theorem (?? I'll try later this).

Solution using complex analysis.

(???? I still don't know how to do it)

Numerical solution.

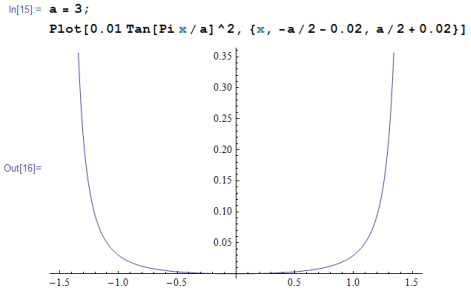
(???? I still don't know how to do it)

Typical. WKB spectrum and number of levels in $V = -U_0 \tan^2\left(\frac{\pi x}{a}\right)$

For the potential $V = -\frac{V_0}{\mathrm{ch}^2\frac{x}{a}}$, determine the energy levels and the total number of discrete levels in the quasi-classical approximation.

Solution by standard integration.

One needs just to do a careful WKB and obtain the integral by some clever method, for example, by differentiation over the parameter.



If we define

$$I(E) = \int\limits_{x_1(E)}^{x_2(E)} \sqrt{2m\left(E - U_0\tan^2\left(\frac{\pi x}{a}\right)\right)}dx,$$

where $x_1(E)$ and $x_2(E)$ are the solution to $E - U_0\tan^2\left(\frac{\pi x}{a}\right) = 0$:

$$x_{1,2} = \mp\frac{a}{\pi}\arctan\left(\sqrt{\frac{E}{U_0}}\right)$$

The minus is here at the top, because it corresponds to the left point, and the plus corresponds to the right one. Using Leibniz integral rule with, in our case $f(E,x) = \sqrt{2m\left(E - U_0\tan^2\left(\frac{\pi x}{a}\right)\right)}$ and, by definition of x_1

and x_2, we have $f\left(E, x_{1,2}(E)\right) = 0$, and we get

$$\frac{dI(E)}{dE} = f\left(E, x_2(E)\right)\frac{d}{dE}x_2(E) - f\left(E, x_1(E)\right)\frac{d}{dE}x_1(E) + \int\limits_{x_1(E)}^{x_2(E)} \frac{\partial}{\partial E} f(E,x)dx$$

$$= 0 + 0 + \sqrt{2m}\int\limits_{x_1(E)}^{x_2(E)} \frac{1}{2}\frac{1}{\sqrt{\left(E - U_0\tan^2\left(\frac{\pi x}{a}\right)\right)}}dx$$

Let us set $z := \sin\left(\frac{\pi x}{a}\right)$, so $dz = \frac{\pi}{a}\cos\left(\frac{\pi x}{a}\right)dx$ and using $\cos\alpha = \sqrt{1-\sin^2\alpha}$ we find $dx = adz/\left(\pi\sqrt{1-z^2}\right)$, also $\tan^2(\pi x/a) = z^2/\left(1-z^2\right)$. Performing the change of variable, we get

$$\frac{dI(E)}{dE} = \frac{\sqrt{2m}}{2}\int\limits_{z_1(E)}^{z_2(E)} \frac{1}{\sqrt{\left(E - U_0\frac{z^2}{1-z^2}\right)}}\frac{a}{\pi}\frac{dz}{\sqrt{1-z^2}} =$$

$$= \frac{a\sqrt{2m}}{2\pi}\int\limits_{z_1(E)}^{z_2(E)} \frac{1}{\sqrt{\left(E - (E+U_0)\,z^2\right)}}dz = \frac{a\sqrt{2m}}{2\pi\sqrt{E}}\int\limits_{z_1(E)}^{z_2(E)} \frac{1}{\sqrt{\left(1 - \frac{E+U_0}{E}z^2\right)}}dz,$$

where $z_{1,2}(E) = \sin\left(\frac{\pi x_{1,2}(E)}{a}\right)$. Then we make another change of variable: $\alpha := \sqrt{\frac{E+U_0}{E}}z$ so $d\alpha = \sqrt{\frac{E+U_0}{E}}dz$, and the integral becomes

$$\frac{dI(E)}{dE} = \frac{a\sqrt{2m}}{2\pi\sqrt{E}}\sqrt{\frac{E}{E+U_0}}\int\limits_{\alpha_1(E)}^{\alpha_2(E)} \frac{d\alpha}{\sqrt{1-\alpha^2}} = \frac{a\sqrt{2m}}{2\pi\sqrt{E+U_0}}\left(\arcsin\alpha_2 - \arcsin\alpha_1\right).$$

The bounds $\alpha_{1,2}$ are defined by

$$\alpha_{1,2} = \sqrt{\frac{E+U_0}{E}}z_{1,2} = \sqrt{\frac{E+U_0}{E}}\sin\left(\frac{\pi x_{1,2}(E)}{a}\right) = \sqrt{\frac{E+U_0}{E}}\sin\left(\frac{\mp\pi\frac{a}{\pi}\arctan\left(\sqrt{\frac{E}{U_0}}\right)}{a}\right)$$

$$= \mp\sqrt{\frac{E+U_0}{E}}\sin\left(\arctan\left(\sqrt{\frac{E}{U_0}}\right)\right).$$

Then by $\sin(\arctan(x)) = \frac{x}{\sqrt{1+x^2}}$ we find

$$\alpha_{1,2} = \mp\sqrt{\frac{E+U_0}{E}}\frac{\sqrt{\frac{E}{U_0}}}{\sqrt{1+\frac{E}{U_0}}} = \mp 1$$

The integral is thus

$$\frac{dI(E)}{dE} = \frac{a\sqrt{2m}}{2\pi\sqrt{E+U_0}}(\arcsin(1) - \arcsin(-1)) = \frac{a\sqrt{2m}}{2\sqrt{E+U_0}}$$

Remembering that $I(0) = 0$, since at $E = 0, x_1 = x_2$, we have

$$I(E) = \sqrt{2m}a\left(\sqrt{E+U_0} - \sqrt{U_0}\right).$$

The energy is then found using $I(E) = \pi\hbar(n+1/2)$:

$$E = \left(\sqrt{U_0} + \frac{\pi\hbar(n+1/2)}{\sqrt{2m}a}\right)^2 - U_0$$

This formula is a combination of the energy of a harmonic oscillator $E = \hbar\omega(n+1/2)$ and of the potential well $E = \hbar^2\pi^2n^2/(2ma^2)$. If we set $U \to 0$, the quasiclassic method does not produce the exact result, but for high n it is a good approximaiton.

Solution using complex analysis.

(???? I still don't know how to do it)

Numerical solution.

(???? I still don't know how to do it)

EK.7.з.1. Turning point

To show that the WKB solution is applicable, the closer to the actual pivot point, the more $U'(x)$ is in it.

Solution.

(порешаю скоро!)

EK.7.з.3. WKB spectrum in the Morse potential

Find the VKB spectrum of a particle in the Morse potential

$$U(x) = U_0 \left(e^{x/a} - 1\right)^2.$$

Solution.

(порешаю скоро!)

17.1.12 Problems about quasiclassics 1: Templates That Require Special Mathematics

EK.7.з.4. ВКБ-спектр в ямке

Найти ВКБ-спектр частицы в потенциале

$$U(x) = -U_0 \operatorname{ch}^{-2}(x/a).$$

Solution.

(порешаю скоро!)

EK.7.з.5 ВКБ-спектр в скругленном колодце

Найти ВКБ-спектр частицы в потенциале

$$U(x) = U_0 \operatorname{tg}^2(\pi x/a), \quad |x| < a/2.$$

Solution.

(порешаю скоро!)

EK.7.з.6. ВКБ-спектр в кривом угле

Найти ВКБ-спектр частицы в потенциале

$$U(x) = U_0 \left(\frac{a}{x} - \frac{x}{a}\right)^2, \quad x > 0.$$

Solution.

(порешаю скоро!)

ЕК.7.з.7. ВКБ-коэффициенты прохождения перевернутого осциллятора (??)

Найти ВКБ-коэффициенты $D(E), R(E)$ в поле с потенциалом

$$U(x) = -\frac{m\omega^2}{2}x^2.$$

Использовать приближение Кембла. Сравнить с точным решением.

ЕК.7.з.8. ВКБ-коэффициенты прохождения бугра

Разложив потенциал

$$U(x) = U_0 \operatorname{ch}^{-2}(x/a)$$

до членов $\sim x^2$, найти ВКБ-коэффициенты $D(E), R(E)$ при $E \approx U_0$, используя результат задачи 7.7. Сравнить с разложением точного решения при $\xi^2 \ll 1$.

ЕК.7.з.9. ВКБ методы для бугра

Найти ВКБ-коэффициент $R(E)$ для частицы в поле

$$U(x) = U_0 \frac{a^2}{a^2 + x^2}.$$

Рассмотреть случаи $U_0 > 0, U_0 < 0$.

ЕК.7.з.10.

Оценить ВКБ-коэффициент прохождения $D(E)$ в поле с потенциалом (рис. 25)

$$\begin{array}{ll} U(x) \approx -U_0 & (x < 0) \\ U(x) \approx -Fx & (x > 0) \end{array}$$

Такой потенциал представляет интерес для описания холодной эмиссии электронов из металла в электрическом поле напряженности F. Величина U_0 соответствует работе выхода.

Б-2.7.1 Квазиклассика в осцилляторе и обрезанном осцилляторе

Найти в квазиклассическом приближении уровни энергии и собственные функции:
а) линейного гармонического осциллятора;
б) частицы, движущейся в поле

$$U(x) = \begin{cases} \infty, & x \leqslant 0 \\ \frac{m\omega^2 x^2}{2} & x > 0 \end{cases}$$

(add picture)

а) решение в осцилляторе

Исходя из правила квантования Бора-Зоммерфельда, имеем

$$\int\limits_a^b p(x)dx = \int\limits_{-x_0}^{x_0} \sqrt{2mE - m^2\omega^2 x^2}dx = \pi\hbar\left(n + \frac{1}{2}\right),$$

где $x_0 = \sqrt{2E/(m\omega^2)}$ - классическая точка поворота. Вычисляя интеграл (1), получим $E\pi/\omega$, откуда найдем уровни энергии:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, ...$$

Построим волновую функцию, исходя из правила согласования квазиклассических решений при переходе из классически запрещенной области в классически разрешенную (II.36):

$$\psi_n(x) = C \begin{cases} \frac{(-1)^n}{2\sqrt{|p(x)|}} \exp\{-z_1\}, & x < -a \\ \frac{1}{\sqrt{p(x)}} \sin\{z_2 + \pi/4\}, & -a < x < a \\ \frac{1}{2\sqrt{|p(x)|}} \exp\{-z_3\}, & x > a \end{cases}$$

$$z_1 := \frac{1}{\hbar}\int\limits_x^{-a} |p(\xi)|d\xi, \quad z_2 := \frac{1}{\hbar}\int\limits_{-a}^{a} p(\xi)d\xi, \quad z_3 := \frac{1}{\hbar}\int\limits_a^{x} |p(\xi)|d\xi.$$

При расчете нормировочного множителя, как и обычно, пренебрегаем вкладом экспонент и считаем, что $\sin^2\alpha = 1/2$ (функция быстро осциллирует), поэтому $C \simeq \sqrt{2m\omega/\pi}$.

(check!!!)

Вычисляя интегралы, окончательно получаем (check!!!)

$$z_2 = \frac{E_n}{\hbar\omega}\left[\frac{x}{x_0}\sqrt{1-\left(\frac{x}{x_0}\right)^2} + \arcsin\left(\frac{x}{x_0}\right) + \frac{\pi}{2}\right],$$

$$z_{1,3} = \frac{E_n}{\hbar\omega}\left[\mp\frac{x}{x_0}\sqrt{\left(\frac{x}{x_0}\right)^2 - 1} - \ln\left(\mp\frac{x}{x_0} + \sqrt{\left(\frac{x}{x_0}\right)^2 - 1}\right)\right].$$

The prefactor is

$$\frac{C}{2\sqrt{|p(x)|}} \simeq \frac{1}{\sqrt{2\pi\sqrt{x^2 - x_0^2}}}, \qquad \frac{C}{\sqrt{p(x)}} \simeq \sqrt{\frac{2}{\pi\sqrt{x_0^2 - x^2}}}.$$

(x_0 was introduced in the beginning, it is a turning point)

(write the final formula)

б) решение в обрезанном осцилляторе (!?!!!)

(!!! нужно еще раз про модификацию БЗ прописать и продумать!)

Прежде всего заметим, что условия применимости метода ВКБ (плавный ход потенциала взаимодействия) выполняются вплоть до $x = 0$, а в точке $x = 0$ необходимо поставить граничное условие $\psi(0) = 0$ (рис. 2.8).

Поэтому должно выполняться условие (для классически разрешенной области)

$$\sin\left\{\frac{1}{\hbar}\int\limits_0^{x_0} p(x)dx + \frac{\pi}{4}\right\} = 0$$

что приводит к модификации правила квантования Бора-Зоммерфельда:

$$\int\limits_0^{x_0} p(x)dx = \pi\hbar\left(n + \frac{3}{4}\right).$$

Из соотношения (3) получаем уровни энергии:

$$E_n = \hbar\omega\left(2n + \frac{3}{2}\right), \quad n = 0, 1, 2...$$

которые совпадают с нечетными уровнями для случая а).

Thuus, the wave functions are the $\widetilde{\psi}_n(x)$ for the oscillator, but only the odd ones, and only in the positive side (which is allowed by the potential). They were normalized, so since now we have half of them, then square of them equal to one, so the final wave function look like this:

$$\widetilde{\psi}_n(x) = \begin{cases} \sqrt{2}\psi_{2n+1}(x), & x > 0, \\ 0, & x \leqslant 0. \end{cases}$$

(write the final formulas)

17.1.13 Problems about quasiclassical method 2

Б-2.7.2 Спектр в угле

Найти в квазиклассическом приближении уровни энергии и собственные функции частицы в поле

$$U(x) = \begin{cases} \infty, & x \leqslant 0 \\ Fx, & x > 0 \end{cases}$$

Solution.

В данной задаче, как и в задаче 2.7.1 п. б) необходимо поставить специальное граничное условие при $x = 0$, т. е. $\psi(0) = 0$. Это приводит к следующему виду правила квантования:

$$\int\limits_0^{x_0} p(\xi)d\xi = \int\limits_0^{E/F} \sqrt{2m(E - F\xi)}d\xi = \pi\hbar\left(n + \frac{3}{4}\right).$$

В итоге получаем энергетические уровни:

$$E_n = \left(\frac{3\pi\hbar F}{2\sqrt{2m}}\right)^{2/3}\left(n + \frac{3}{4}\right)^{2/3}$$

и согласованные квазиклассические функции. В классически разрешенной области функция имеет вид

$$\psi_n(x)|_{0<x<\frac{E_n}{F}} = \left(\frac{F^2}{E_n - Fx}\right)^{1/4}\sin\left\{\frac{2\sqrt{2m}}{3F\hbar}\left(E_n - Fx\right)^{3/2} + \frac{\pi}{4}\right\},$$

и в классически запрещенной:

$$\psi_n(x)|_{x>\frac{E_n}{F}} = \frac{1}{2}\left(\frac{F^2}{Fx - E_n}\right)^{1/4}\exp\left\{-\frac{2\sqrt{2m}}{3F\hbar}\left(Fx - E_n\right)^{3/2}\right\}.$$

Б-2.7.3 Закон Гейгера-Неттола

Найти в квазиклассическом приближении коэффициент прохождения через потенциальный барьер

$$U(x) = \begin{cases} -U_0, & x \leqslant r_0 \\ \frac{2Ze^2}{x}, & x > r_0. \end{cases}$$

Получить приближенное выражение для коэффициента прохождения, считая, что $r_0 \ll 2Ze^2/E$. Обсудить связь этой задачи с элементарной теорией альфа-распада и получить закон Гейгера-Неттола.

Solution.

(! в 1ю часть в типичные модели про это напишу!)
Согласно формуле Гамова (II.38) коэффициент прохождения через потенциальный барьер равен

$$D \simeq \exp\left\{-\frac{2}{\hbar}\int\limits_a^b |p(x)|dx\right\},$$

где

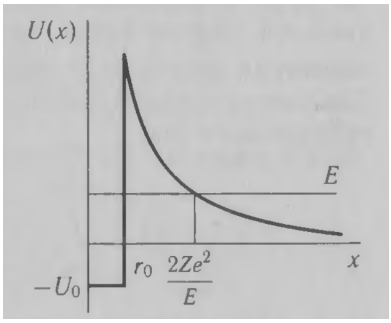
$$\int\limits_a^b |p(x)|dx = \int\limits_a^b \sqrt{2m(U(x) - E)}dx = \sqrt{2m}\int\limits_{r_0}^{2Ze^2/E}\sqrt{\frac{2Ze^2}{x} - E}dx.$$

Вычисляя интеграл, получаем

$$D \simeq \exp\left\{-\frac{4Ze^2}{\hbar}\sqrt{\frac{2m}{E}}(\arccos\sqrt{\alpha} - \sqrt{\alpha(1-\alpha)})\right\},$$

где $\alpha = \frac{r_0 E}{2Ze^2}$. В случае, если $\alpha \ll 1$, выражение (1) упрощается:

$$D \simeq \exp\left\{-\frac{2\pi Ze^2}{\hbar}\sqrt{\frac{2m}{E}}\right\}.$$



Следует заметить, что выражения (1) и (2) определяют коэффициент прохождения лишь по порядку величины, т. е. показывают его экспоненциальную малость. Поскольку условия применимости метода ВКБ нарушаются в точке $x = r_0$ (резкий скачок потенциала), то условия сшивания решений в данной точке требуют уточнения. В точном выражении в отличие от (2) появляется предэкспоненциальный множитель ~ 1.

Данная задача рассматривалась впервые в связи с теорией α-распада. С точки зрения квантовой механики α-распад представляет собой типичное явление прохождения частицы через потенциальный барьер.

Итак, α-частица вначале «заперта» в области $x \leqslant r_0$ (зона действия потенциала притяжения ядра, рис. 2.9). Для того, чтобы выйти из ядра, т. е. излучиться, α-частица должна преодолеть потенциальный барьер (при $x > r_0$ на частицу будут действовать кулоновские силы отталкивания).

Вероятность α-распада (или прохождения через барьер) в единицу времени λ пропорциональна коэффициенту прохождения D : $\lambda = nD$, где n - число столкновений со стенкой барьера в единицу времени.

Величину n можно оценить следующим образом: $n \sim v/r_0$, где v - характерная скорость частицы в потенциальной яме. Далее

$$v \sim \frac{p}{m_\alpha} \sim \frac{\hbar}{m_\alpha r_0}, \quad \text{поэтому } n \sim \frac{\hbar}{m_\alpha r_0^2}.$$

Период полураспада $T_{1/2}$ связан с вероятностью распада в единицу времени λ известным соотношением:

$$T_{1/2} = \frac{\ln 2}{\lambda} \simeq \frac{m_\alpha r_0^2 \ln 2}{\hbar D} = C_1 \exp\left[\frac{C_2}{\sqrt{E}}\right],$$

где последнее равенство является следствием (2). Логарифмируем (3) и получаем соотношение

$$\ln T_{1/2} = A + \frac{B}{\sqrt{E}},$$

которое и представляет собой закон Гейгера-Неттола. Величины A и B, разумеется, несложно выразить через исходные данные задачи.

Б-2.7.4

Найти в квазиклассическом приближении коэффициент прохождения через потенциальный барьер

$$U(x) = \begin{cases} 0, & |x| > x_0, \\ U_0 - \frac{m\omega^2 x^2}{2}, & |x| < x_0, \end{cases}$$

при условии $0 < E < U_0$.

Solution.

2.7.4. $D \simeq \exp\left\{-\frac{2\pi(U_0 - E)}{\hbar\omega}\right\}$.

Б-2.7.5

Исходя из правила квантования Бора-Зоммерфельда, получить выражение для смещения энергетических уровней частицы при изменении потенциальной энергии на малую величину $\delta U(x)$.

Solution.

2.7.5. Пусть возмущенный потенциал имеет вид $U(x) = U_0(x) + \delta U(x)$, где $U_0(x)$ - начальный потенциал, а $U(x)$ - малое изменение потенциальной энергии. Будем считать, что дискретные уровни энергии при наложении возмущения изменяются по схеме: $E_n^{(0)} \to E_n = E_n^{(0)} + \delta E_n$. Для поиска поправки δE_n представим формулу квантования Бора-30ммерфельда в виде

$$\pi\hbar\left(n+\frac{1}{2}\right) = \int\limits_{a+\delta a}^{b+\delta b} \sqrt{2m\left(E_n^{(0)} + \delta E_n - U_0(x) - \delta U(x)\right)}dx$$

где δa и δb характеризуют возможные сдвиги точек поворота. Очевидно, что должно выполняться

$$U_0(a+\delta a) + \delta U(a) = E_n^{(0)} + \delta E_n,$$

откуда легко получить, что

$$|\delta a| = |\frac{\delta E_n - \delta U(a)}{U'(a)}| \ll 1,$$

т. е. $|\delta a| \ll 1$ и $|\delta b| \ll 1$, если выполнены условия квазиклассичности. Нетрудно показать, что изменение интеграла за счет сдвига точек поворота $\sim (\delta a)^{3/2}$ (или $\sim (\delta b)^{3/2}$), и в линейном приближении соответствующие поправки должны быть отброшены. Поэтому оставляем в интеграле (1) в пределах интегрирования только a и b, и, проводя разложение подынтегрального выражения с линейной точностью по $\delta U(x)$, δE_n, получаем

$$\delta E_n \simeq \int\limits_a^b \frac{\delta U(x)dx}{\sqrt{2m\left(U_0(x) - E_n^{(0)}\right)}} / \int\limits_a^b \frac{dx}{\sqrt{2m\left(U_0(x) - E_n^{(0)}\right)}} = \frac{2}{T}\int\limits_a^b \frac{\delta U(x)dx}{v_0(x)},$$

где T - полный период классического движения частицы в потенциале $U_0(x)$, $v_0(x)$ - классическая скорость частицы.

Данный результат может быть получен и в первом приближении теории возмущений, если в качестве невозмущенной функции взять квазиклассическую функцию. В этом случае при расчете интегралов нужно пренебречь вкладом экспонент и заменить квадрат синуса на 1/2 под знаком интеграла, считая, что функция быстро осциллирует.

ПТФ-11.y1. Другие задачи сшивки

Найдите квазиклассические уровни энергии для следующих потенциалов, и сравните полученные ответы с уже известными.

• треугольная яма $U(x) = \begin{cases} +\infty, x < 0, \\ Fx, x > 0. \end{cases}$

• трёхмерный кулоновский потенциал $U(r) = -\frac{e^2}{r}$ для сферически симметричных состояний.

Указание: определите граничное условие в нуле, а в правой точке остановки используйте стандартное. Обратите внимание, что в этих задачах в одной из точек остановки линейное приближение для потенциала неприменимо, поэтому условие сшивки необходимо модифицировать. Для второй задачи вам может помочь упражнение 5.2.

Solution. Треугольный потенциал

Волновая функция в квазиклассике:

$$\psi(x) = \frac{1}{\sqrt{p(x)}}\cos\left(\int\limits_b^x p(y)dy - \frac{\pi}{4}\right)$$

где b – правая точка остановки. Условие непрерывности волновой функции в нуле

$$\psi(0) = 0$$

дает условие квантования Бора-Зоммерфельда:

$$\int\limits_a^b p(y)dy + \frac{\pi}{4} = \pi n - \frac{\pi}{2}, \quad p(x) = \sqrt{2m(E-Fx)}$$

(???? перевыведу формулу ниже, в теории она должна быть уже, где нули функции Айри.)

$$E_n = \left(\frac{3\pi F}{2\sqrt{2m}}\left(n - \frac{3}{4}\right)\right)^{2/3}$$

Solution. Кулоновский потенциал

(???? не уверен, насколько это решение верное. непонятно, откуда взялся $\nu = 1/2s$. Интегралы непонятно как взяты. Плохо решена задача, переделывать нужно!)

Поскольку рассматриваются сферически-симметричные состояния, то $l = m = 0$.

В упражнении 5.2. мы нашли решение для кулоновского потенциала для $E = 0$:

$$\psi(r,\theta,\phi) = J_{2l+1}\left(2\sqrt{\frac{2M\alpha}{\hbar^2}r}\right)\left(\sqrt{\frac{2M\alpha}{\hbar^2}r}\right)^{-1}\mathcal{Y}_{l,m}(\theta,\phi)$$

$$-\frac{\hbar^2}{2m}u''(r) - \frac{e^2}{r}u(r) = Eu(r), \quad \psi_{l,m}(r,\theta,\varphi) = R_E(r)\mathcal{Y}_{l,m}(\theta,\varphi), \quad R(r) = \frac{u(r)}{r}$$

Применим квазиклассическое приближение к этому уравнению. Волновая функция ограничена, а значит $u(r) \to 0$ при $r \to 0$. Т.е. все решения при малых r эквивалентны ассимтотически решению на нулевой энергии, поскольку совпадают стационарные уравнения Шрёдингера:

$$\frac{\hbar^2}{2m}u''(r) - \frac{e^2}{r}u(r) = 0$$

Поскольку в правой точке нужно использовать стандартное граничное условие, то

$$u(r) = \frac{1}{\sqrt{p(r)}}\cos\left(\int\limits_b^r p(r)dr - \frac{\pi}{4}\right), \quad p(r) = \sqrt{2m\left(E + \frac{e^2}{r}\right)}$$

где b - правая точка остановки. Сшиваем решение для нулевой энергии с квазиклассическим решением, где они оба применимы. Ассимптотика функции Бесселя:

$$J_\nu(z) \approx \sqrt{\frac{2}{\pi z}}\cos\left(z - \frac{\pi\nu}{2} - \frac{\pi}{4}\right), \quad z \to \infty$$

$$u(r) \sim r^{1/4}\cos\left(2\sqrt{\frac{2M\alpha}{\hbar^2}r} - \frac{\pi}{4} - \frac{\pi}{2}\right)$$

But from another side,

$$u(r) = \frac{1}{\sqrt{p(r)}}\cos\left(\int\limits_0^r p(r)dr + \phi\right)$$

$$\int\limits_0^r p(r)dr = \sqrt{2m}\int\limits_0^r \sqrt{E + \frac{e^2}{r}}dr \approx 2\sqrt{2me^2}\sqrt{r}$$

$$\phi = -\frac{3\pi}{4} \equiv \frac{\pi}{2} \qquad \text{(since under cos)}$$

Условие квантования:

$$\int\limits_0^b p(r)dr = \pi\hbar n$$

$$\int\limits_0^b p(r)dr = \sqrt{2me^2}\cdot\int\limits_0^b \sqrt{\frac{1}{r}-\frac{1}{b}}dr \overset{\text{wlf}}{=} \int\limits_0^b p(r)dr = \sqrt{2me^2}\cdot\frac{\pi}{2}\sqrt{b}$$

(?? что-то рукой не поситал его, потом поупражняюсь еще. попробовал заменить всё под корнем как новую переменную, но пока не увидел, к какому интегралу сводится он, что аж π вылазит)

$$\sqrt{2me^2 b_n}\frac{\pi}{2} = \pi\hbar n$$

$$E_n = -\frac{me^4}{2\hbar^2 n^2}$$

Получился точный ответ для уровней энергии!

ПТФ-11.y2

Рассмотрите $N(E)$ – количество состояний с энергией, меньше заданной E в поле произвольного адекватного трехмерного сферически-симметричного потенциала $U(r)$ в рамках квазиклассического приближения. Покажите, что следующие два способа вычисления приводят к одному и тому же результату а) одномерное правило квантования Бора-Зоммерфельда для радиальной переменной (отдельно для каждой сферической гармоники) с последующим суммированием по гармоникам и б) использование интеграла по трехмерному фазовому объему: $N(E) = \int d^3r \int \frac{d^3p}{(2\pi\hbar)^3}\theta(E-E_p)$, где $E_p = \frac{p^2}{2m}$.

[а)] Уравнение Шредингера для радиальной переменной

$$-\frac{\hbar^2}{2M}u''(r) + U'(r)u(r) = Eu(r), \quad u(r) = rR_E(r), \quad U'(r) = U(r) + \frac{l(l+1)}{2Mr^2}$$

Одномерное правило квантования Бора-Зоммерфельда:

$$\int\limits_{r^l_{\min}}^{r^l_{\max}} \sqrt{2M(E_{n,l,m} - U'(r))}dr = \pi\hbar\left(n+\frac{1}{2}\right)$$

Обозначим через $N_{E,l}$ – максимальное n, для которого $E_{n,l,m} \le E$.

$$\int\limits_{r^l_{\min}}^{r^l_{\max}} \sqrt{2M(E - U'(r))}dr = \pi\hbar\left(N_{E,l}+\frac{1}{2}\right)$$

$$\begin{aligned}
N(E) &= \sum_m \sum_{l=0}^{l_{\max}} N_{E,l} = \sum_{l=0}^{l_{\max}} (2l+1)N_{E,l} = \\
&= \int\limits_0^{l_{\max}} dl(2l+1)\frac{\sqrt{2M}}{\pi\hbar}\int\limits_{r^l_{\min}}^{r^l_{\max}} \sqrt{E - U(r) - \frac{l(l+1)}{2Mr^2}}dr = \\
&= -\frac{\sqrt{2M}}{\pi\hbar}\frac{4M}{3}\int\limits_{r_{\min}}^{r_{\max}} drr^2\left(E - U(r) - \frac{l(l+1)}{2Mr^2}\right)^{3/2}\Bigg|_{l=0}^{l=l_{\max}} \overset{\text{only } l=0}{=} \\
&= \frac{2(2M)^{3/2}}{3\pi\hbar}\int\limits_{r_{\min}}^{r_{\max}} r^2(E-U(r))^{3/2}dr
\end{aligned}$$

[б)] Интеграл по трёхмерному фазовому объёму:

$$N(E) = \int d^3r \int \frac{d^3p}{(2\pi\hbar)^3}\theta(E - E_p) = \int d^3r \int\limits_0^{p_{\max}} \frac{dp 4\pi p^2}{(2\pi\hbar)^3}$$

$$p_{\max} = \sqrt{2m(E - U(\vec{r}))}$$

$$N(E) = \frac{4\pi(2m)^{3/2}}{3(2\pi\hbar)^3}\int d^3r (E - U(r))^{3/2} = \frac{2(2m)^{3/2}}{3\pi\hbar}\int\limits_{r_{\min}}^{r_{\max}} dr r^2 (E - U(r))^{3/2}$$

ПТФ-11.у3 Туннелирование под $\frac{1}{\cosh^2(x/a)}$

Найдите вероятность квазиклассического туннелирования под барьером $U(x) = \frac{U_0}{\cosh^2(x/a)}$ для частиц энергии $0 < E < U_0$. Сравните ответ с точным (?допишу формулу).

Solution.

Общий вид волновой функции в квазиклассическом приближении:

$$\psi(x) = c_+\psi_+(x) + c_-\psi_-(x), \quad \psi_\pm(x) = \frac{e^{\pm i\int\limits_{x_0}^{x} p(x)dx}}{\sqrt{p(x)}}$$

Задача рассеяния:

$$\psi(x) = \begin{cases} \frac{1}{\sqrt{p(x)}}e^{i\int\limits_0^x p(z)dz} + \frac{r}{\sqrt{p(x)}}e^{-i\int\limits_0^x p(z)dz}, & x < 0 \\ \frac{t}{\sqrt{p(x)}}e^{i\int\limits_0^x p(z)dz}, & x > 0 \end{cases}$$

Это решение переписывается в следующем виде:

$$\psi(x) = \begin{cases} \psi_+(x) + r\psi_-(x), & x < 0 \\ t\psi_+(x), & x > 0 \end{cases}$$

Связь на коэффициенты:

$$\begin{pmatrix} c^+_{\text{left}} \\ c^-_{\text{left}} \end{pmatrix} = \hat{A}\hat{S}\hat{A}^\dagger \begin{pmatrix} c^+_{\text{right}} \\ c^-_{\text{right}} \end{pmatrix}, \quad \hat{A} = \begin{pmatrix} \frac{e^{-\frac{i\pi}{4}}}{2} & e^{\frac{i\pi}{4}} \\ \frac{e^{\frac{i\pi}{4}}}{2} & e^{-\frac{i\pi}{4}} \end{pmatrix}, \quad \hat{S} = \begin{pmatrix} e^{-S} & 0 \\ 0 & e^{S} \end{pmatrix}$$

$$\hat{A}\hat{S}\hat{A}^\dagger = \begin{pmatrix} \frac{1}{4}e^{-S} + \frac{1}{2}e^{S} & -\frac{i}{2}e^{-S} + ie^{S} \\ \frac{i}{4}e^{-S} - \frac{i}{2}e^{S} & \frac{1}{2}e^{-S} + e^{S} \end{pmatrix}$$

$$\begin{pmatrix} c^+_{\text{right}} \\ c^-_{\text{right}} \end{pmatrix} = \begin{pmatrix} 0 \\ t \end{pmatrix} \to \begin{pmatrix} c^+_{\text{left}} \\ c^-_{\text{left}} \end{pmatrix} = \begin{pmatrix} 1 \\ r \end{pmatrix} = t\begin{pmatrix} -\frac{i}{2}e^{-S} + ie^{S} \\ \frac{1}{2}e^{-S} + e^{S} \end{pmatrix}$$

$$t = \frac{i}{\frac{e^{-S}}{2} - e^{S}}, \quad r = i\frac{e^{-S} + 2e^{S}}{e^{-S} - 2e^{S}}$$

$$T = (\frac{e^{-S}}{2} - e^{S})^{-2}$$

Точки остановки:

$$\frac{U_0}{\cosh^2(x_{1,2}/a)} = E \to x_{1,2} = a\,\text{arccosh}\left(\pm\sqrt{\frac{U_0}{E}}\right)$$

$$S = \int\limits_{x_1}^{x_2}\sqrt{2m(U(x) - E)}dx = \sqrt{2m}\pi a(\sqrt{U_0} + \sqrt{E})$$

$$T = \left(\frac{e^{-\sqrt{2m}\pi a(\sqrt{U_0}+\sqrt{E})}}{2} - e^{\sqrt{2m}\pi a(\sqrt{U_0}+\sqrt{E})}\right)^{-2}$$

(!! тут скорее всего большая халтура, интеграл то не считается так просто! а у меня где-то в этом файле приведено решение его, впишу)

ПТФ-11.y4 Нормировка в квазиклассике

• Отнормируйте волновые функции связанного состояния, которые следуют из правила квантования Бора-Зоммерфельда, на единицу.
• Отнормируйте квазиклассические бегущие волны (в отсутствие отражения) на $2\pi\delta(E-E_0)$

Solution.

• Волновые функции для частицы в потенциальной яме:

$$\psi(x)=\frac{C}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\int\limits_a^x p(y)dy-\frac{\pi}{4}\right)$$

Условие нормировки:

$$\int\limits_a^b|\psi(x)|^2dx=\int\limits_a^b\frac{C^2}{p(x)}\cos^2\left(\frac{1}{\hbar}\int\limits_a^x p(y)dy-\frac{\pi}{4}\right)dx=1$$

Импульс меняется медленно, а косинус между точками остановки успевает совершить достаточно много колебаний. Поэтому, заменим $\cos^2$ на среднее значение за период.

$$\frac{C^2}{2}\int\limits_a^b\frac{dx}{p(x)}=1$$

Стоящий здесь интеграл выражается через период колебаний классической частицы в этом же потенциале:

$$T=2\int\limits_a^b\frac{dx}{v(x)}=2m\int\limits_a^b\frac{dx}{p(x)}dx\to C=\sqrt{\frac{4m}{T}}$$

$$\psi(x)=\sqrt{\frac{4m}{Tp(x)}}\cos\left(\frac{1}{\hbar}\int\limits_a^x p(y)dy-\frac{\pi}{4}\right)$$

• Квазиклассические бегущие волны:

$$\psi_\pm(x)=\frac{C}{\sqrt{p(x)}}\exp\left(\pm\frac{i}{\hbar}\int\limits_0^x p(y)dy\right)$$

$$\langle\psi_+^E|\psi_+^{E'}\rangle=C^2\int\limits_{-\infty}^{\infty}\frac{e^{\frac{i}{\hbar}\int\limits_0^x(p^{E+\delta E}(y)-p^E(y))dy}}{p^E(x)}dx$$

$$p^{E+\delta E}(y)-p^E(y)\approx\frac{\partial p^E(y)}{\partial E}\delta E=\frac{m}{p(y)}\delta E$$

Пусть $\xi=\frac{m}{\hbar}\int\limits_0^x\frac{dy}{p(y)}$, тогда

$$\langle\psi_+^E|\psi_+^{E'}\rangle=C^2\frac{m}{\hbar}\int\limits_{-\infty}^{\infty}e^{i\xi\delta E}d\xi=C^2\frac{m}{\hbar}2\pi\delta(E'-E)$$

Для перекрекстных скалярных произведений:

$$\langle\psi_+^E|\psi_-^{E'}\rangle=C^2\frac{m}{\hbar}\int\limits_{-\infty}^{\infty}e^{i\xi(E+E')}d\xi=C^2\frac{m}{\hbar}2\pi\delta(E'+E)\approx0$$

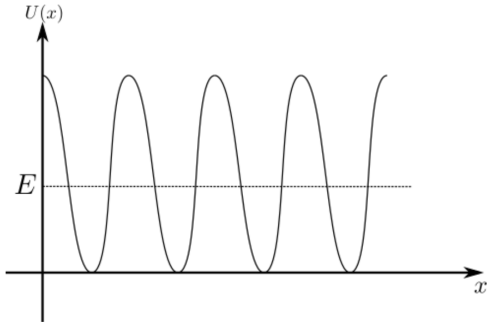
Таким образом, нормированные на дельта-функцию квазиклассические бегущие волны:

$$\psi_\pm(x)=\sqrt{\frac{\hbar}{2\pi mp(x)}}\exp\left(\pm\frac{i}{\hbar}\int\limits_0^x p(y)dy\right)$$

ПТФ-11.з2. Одномерный кристалл и модель сильной связи

Определите зоны и их законы дисперсии для периодической задачи, изображённой на рисунке, считая применимым квазиклассическое приближение. Проинтерпретируйте результат в терминах модели сильной связи и следующего гамильтониана (для каждой зоны). Определите E_n и t_n.

$$\hat{H}_n = \begin{pmatrix} \ddots & -t_n & 0 & 0 & \dots \\ -t_n & E_n & -t_n & 0 & 0 \\ 0 & -t_n & E_n & -t_n & 0 \\ 0 & 0 & -t_n & E_n & -t_n \\ \vdots & 0 & 0 & -t_n & \ddots \end{pmatrix}$$



Solution.

Рассмотрим кристалл из очень большого, но все же конечного количества атомов $N \gg 1$.

$$\hat{Q} = \hat{A}^\dagger \begin{pmatrix} e^{-iS} & 0 \\ 0 & e^{iS} \end{pmatrix} \hat{A} \begin{pmatrix} e^{-S_T} & 0 \\ 0 & e^{S_T} \end{pmatrix}, \quad \hat{A} = \begin{pmatrix} \frac{e^{-i\pi/4}}{2} & e^{i\pi/4} \\ \frac{e^{i\pi/4}}{2} & e^{-i\pi/4} \end{pmatrix}$$

На границах кристалла потенциал имеет бесконечные стенки, то есть, что частица не может вылететь из кристалла. Тогда, если в кристалле N атомов, то столбцы коэффициентов разложения по квазиклассическим функциям слева и справа имеет вид:

$$\vec{c}_{\text{left}} = \hat{Q}^{N-1} \hat{S} \hat{A} \vec{c}_{\text{right}}$$

Мы рассматриваем состояния частицы, находящейся в кристалле, поэтому выбираем

$$\vec{c}_{\text{left}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \vec{c}_{\text{right}} = \begin{pmatrix} 0 \\ t \end{pmatrix}$$

Характеристический многочлен оператора $\hat{Q}$:

$$\chi_{\hat{Q}}(z) = z^2 - \cos S \left(2e^{S_T} + \frac{1}{2} e^{-S_T} \right) z + 1$$

Произведение собственных чисел $\hat{Q}$ равно 1. Вектор $\vec{c}_{\text{right}}$ раскладывается по обоим собственным векторам, и поэтому если $|\lambda_1| \neq |\lambda_2|$, то существует собственное значение по модулю, большее 1. Но тогда при возведении в очень большую степень норма образа вектора $\vec{c}_{\text{right}}$ будет тожет расти неограниченно. Таким образом,

$$|\lambda_1| = |\lambda_2| = 1 \to \lambda_1 = \lambda = e^{i\varphi}, \lambda_2 = e^{-i\varphi}$$

$$\hat{Q}^{N-1} = \Lambda \begin{pmatrix} e^{i\varphi(N-1)} & 0 \\ 0 & e^{-i\varphi(N-1)} \end{pmatrix} \Lambda^{-1}$$

где Λ – матрица перехода к собственным векторам $\hat{Q}$:

$$\Lambda = \begin{pmatrix} \sin S & \sin S \\ e^{S_T} e^{i\varphi} - \frac{1}{2} \cos S & e^{S_T} e^{-i\varphi} - \frac{1}{2} \cos S \end{pmatrix}$$

$$e^{2i(N-1)\varphi} = 1 \to \varphi_k = \frac{\pi k}{N-1}, \qquad k = 0, ..., 2N-3$$

По теореме Виета:

$$\cos\varphi_k = \cos S e^{S_T}\left(1 + \frac{1}{4}e^{-2S_T}\right) \to \cos S_{n,k} = e^{-S_T}\cos\varphi_k$$

При помощи метода последовательных приближений получаем:

$$E^{(1)}_{n,k} = E^{(0)}_n + (-1)^{n-1}\frac{\hbar\omega}{\pi}\cos\left(\frac{\pi k}{N-1}\right)e^{-\frac{1}{\hbar}\int|p(x)|dx}, \quad k = 0, ..., N-1$$

Рассмотрим модель сильной связи. Система функций:

$$\psi_{n,j}(x) = \begin{cases} \frac{C_{n,j}}{\sqrt{|p(x)|}}e^{-\frac{1}{\hbar}\int\limits_{x_2}^{x} p(x)dx}, & x > x_2 \\ \frac{C_{n,j}}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\int\limits_{x_1}^{x_2} p(x)dx - \frac{\pi}{4}\right), & x_1 < x < x_2. \\ \frac{C_{n,j}}{\sqrt{|p(x)|}}e^{\frac{1}{\hbar}\int\limits_{x_1}^{x} p(x)dx} & x > x_1 \end{cases}$$

где x_1 – левая точка остановки, x_2 – правая.
Нормировочные константы связанных состояний:

$$C_{n,j} = \sqrt{\frac{4\pi}{T_n}}$$

где T_n – классический период колебаний частицы с данной энергией в рассматриваемом потенциале. Тогда

$$t_n = \langle\psi_{n,j+1}|\psi_{n,j}\rangle = \frac{4\pi}{T_n}\int\limits_{-z_0}^{z_0}\frac{dz}{|p(z)|}e^{-\int\limits_{-z_0}^{z_0} p(z)dz}, \quad U(z_0) = E^{(0)}_n$$

ПТФ-10.з.1. Почти квазиклассический потенциал

Определите в квазиклассическом приближении коэффициент отражения частицы энергии E от потенциала, который в некоторой точке x_0 имеет особенность. Исследуйте следующие случаи:
1. Потенциал в точке x_0 испытывает скачок, то есть $U(x_0 - 0) = U_1$ и $U(x_0 + 0) = U_2$.
2. Потенциал в точке x_0 испытывает излом, то есть $U(x < x_0) \approx U_0 - F_1(x - x_0)$ и $U(x > x_0) \approx U_0 - F_2(x - x_0)$.

Solution.

17.1.14 Problems about quasiclassical method 3

ФР. Прохождении лоренцева барьера

В квазиклассическом приближении найти коэффициент прохождения барьера

$$U(x) = \frac{U_0 a^2}{x^2 + a^2}.$$

Обсудить границу применимости решения.

Solution.

$D(E) = \exp\left\{-\frac{2}{\hbar}\int\limits_a^b |p(x,E)|dx\right\}$, тут интеграл заменой $x := a\ \mathrm{sh}\ t$ приводится к виду $\left(\mathrm{sh}\, t_0 = \sqrt{U_0/E - 1} \equiv b^{-1}\right)$ (???)

$$\int\limits_{x_1}^{x_2}|p|dx = 2a\sqrt{2m(U_0 - E)}\int\limits_0^{t_0}\sqrt{1 - \frac{E}{U_0 - E}\,\mathrm{sh}^2\, t}dt.$$

Мы получили эллиптический интеграл второго рода. При $E \ll U_0$ его легко вычислить приближенно, если учесть, что при этом подкоренное выражение равно единице во всем интервале интегрирования, за исключением узкой области вблизи верхнего предела интегрирования, в которой $\operatorname{sh} t \gg 1$, и поэтому можно положить во всем интервале интегрирования $\operatorname{sh}^2 t \approx e^{2t}/4$, так что интеграл принимает вид

$$I = \int\limits_0^t \sqrt{1 - b^2 \operatorname{sh}^2 t} dt \approx \int\limits_0^t \sqrt{1 - \frac{b^2}{4} e^{2t}} dt$$

Этот же интеграл с помощью замены переменной $(b/2)e^t = \sin z$ легко вычисляется и при $(b \ll 1)$

$$I = -1 + \ln \left[4\sqrt{U_0/E} \right].$$

Таким образом,

$$D(E) \approx \left(\frac{E}{16U_0} \right)^{\frac{2}{\hbar} a\sqrt{2mU}} \exp\left(\frac{4}{\hbar} a\sqrt{2mU_0} \right).$$

О границах применимости решения

Для справедливости полученного результата требуется выполнение двух условий:
1) $|d\lambda(x)/dx| \ll 1$ во всей области переменной x, за исключением узких интервалов, непосредственно примыкающих к точкам поворота;
2) расстояния $\Delta x_{1,2} \equiv (x - x_{1,2})$ от точек поворота, на которых уже выполняются условия применимости квазиклассики $|d\lambda/dx| \ll 1$, должны быть такими, чтобы при этом можно было ограничиться линейным разложением потенциальной энергии

$$U(x) \approx U(x_{1,2}) + U'(x_{1,2}) \Delta x_{1,2}$$

(при дальнейшем увеличении $|\Delta x_{1,2}|$ выполнения условия линейного разложения, конечно, не требуется).
В рассматриваемой задаче при $|x| > a$ имеем $|d\lambda/dx| \equiv \equiv 0 \ll 1$. При $|x| < a$

$$\left|\frac{d\lambda}{dx}\right| = \frac{\hbar U_0 |x|}{\sqrt{2m} a^2 |E - U(x)|^{3/2}} = \frac{\hbar |x| a}{\sqrt{2m U_0} |x^2 - x_0^2|^{3/2}},$$

и в случае

$$\sqrt{mU_0 a^2/\hbar^2} \gg 1$$

выражение $|\frac{d\lambda}{dx}|$ много меньше единицы при всех значениях x, за исключением узких областей в окрестности точек поворота, причем ширина области неквазиклассичности по порядку величины равна

$$\Delta x = |x - x_{1,2}| \sim \frac{\hbar^{2/3} a^{1/3}}{m^{1/3}} \frac{1}{U_0^{1/6} (U_0 - E)^{1/6}}$$

(для получения этой оценки Δx в выражении $|\frac{d\lambda}{dx}|$ следует положить $|x| \approx x_0$ и $|x^2 - x_0^2| \equiv |x^2 - x_{1,2}^2| = |(x - x_{1,2})(x + x_{1,2})| \approx \approx 2\Delta x x_0$). Применимость квазиклассики требует выполнения оче видного неравенства

$$\Delta x \ll x_0, \quad \text{или } \frac{(U_0 - E) a\sqrt{m}}{\hbar\sqrt{U_0}} \gg 1$$

(в противном случае в интервале между точками поворота $|x| < x_0$ условия применимости квазиклассики не выполнены ни при каких значениях x). Условие $\frac{(U_0 - E) a\sqrt{m}}{\hbar\sqrt{U_0}} \gg 1$ дает, согласно формуле для D, $D \ll 1$, что, как известно, является необходимым (но не доста точным!) условием применимости квазиклассического рассмотрения.
Т.о. для данной задачи условиями применимости полученного результата являются

$$\frac{a}{\hbar}\sqrt{2mU_0} \gg 1, \quad E \ll \frac{\hbar}{a}\sqrt{\frac{U_0}{m}},$$

первое из которых обеспечивает применимость квазиклассики. Второе же заменяет условие $E \ll U_0$, использованное при вычислении интеграла в самом начале. Причина этой замены состоит в том, что при приближенном расчете величины f вида $f = e^A$, когда приближенно вычисляется значение A, для того чтобы было выполнено условне $f_{\text{точн}}/f_{\text{прибл}} \approx 1$, требуется $|A_{\text{точн}} - A_{\text{прибл}}| \ll 1$ (а не просто $A_{\text{точн}}/A_{\text{прибл}} \approx 1$, и это обстоятельство следует учитывать в случае $|A| \gg 1$). И именно второе из этих условий (а не условие $E \ll U_0$) обеспечивает справедливость полученного значения коэффициента прохождения.

Киселев-6.1. Осциллятор с $\delta V = \epsilon m^2\omega^3 x^4/\hbar$ квазиклассикой

Вычислить поправку к энергии осциллятора за счет возмущения $\delta V = \epsilon m^2\omega^3 x^4/\hbar$, где $\epsilon \to 0$, и определить условие применимости метода теории возмущений для конечных значений ϵ.

Solution.

(?? казалось бы, причем тут квазиклассика?? видно, не усвоил еще. укажу в теории, чтобы очевидно это было!!!)

Согласно общему правилу квантования Бора-Зоммерфельда, спектр невозмущенного осциллятора задается условием

$$\oint p_0(x)\mathrm{d}x = 2\pi\hbar\left(n+\frac{1}{2}\right), \quad p_0(x) = \sqrt{2m\left(E_n^{(0)} - \frac{m\omega^2 x^2}{2}\right)},$$

так что с помощью замены $x = \sqrt{\frac{2E_n^{(0)}}{m\omega^2}}\sin\phi$ находим

$$\oint p_0(x)\mathrm{d}x = \frac{2E_n^{(0)}}{\omega}\int\limits_0^{2\pi}\cos^2\phi\mathrm{d}\phi = \frac{2\pi}{\omega}E_n^{(0)}.$$

В итоге спектр осциллятора в квазиклассике

$$E_n^{(0)} = \hbar\omega\left(n+\frac{1}{2}\right)$$

совпадает с точным выражением.

Поправку к энергии

$$\delta E_n = \frac{\oint \frac{\mathrm{d}x}{p_0}\delta V(x)}{\oint \frac{\mathrm{d}x}{p_0}}$$

определяют

$$\oint \frac{\mathrm{d}x}{p_0} = \frac{1}{m\omega}\int\limits_0^{2\pi}\mathrm{d}\phi = \frac{2\pi}{m\omega}$$

$$\oint \frac{\mathrm{d}x}{p_0}\delta V(x) = \epsilon\frac{4\left(E_n^{(0)}\right)^2}{m\omega^2\hbar}\int\limits_0^{2\pi}\sin^4\phi\mathrm{d}\phi = \frac{3}{2}\epsilon\frac{2\pi h}{m}\left(n+\frac{1}{2}\right)^2.$$

В итоге

$$\delta E_n = \frac{3}{2}\epsilon\hbar\omega\left(n+\frac{1}{2}\right)^2.$$

Критерий применимости теории возмущений в квазиклассике, $\delta E \ll \hbar\omega$, дает

$$\epsilon\cdot n^2 \ll 1 \text{ при условии } n \gg 1.$$

Отсюда, между прочим, следует, что требование точности вычислений по теории возмущений в квазиклассике на уровне, скажем, порядка нескольких процентов при конечном значении параметра малости $\epsilon \sim 0,1$ может оказаться совершенно недостижимым, поскольку для этого квантовое число n должно принимать слишком малые значения, что недопустимо в квазиклассическом приближении.

Комбинированный критерий применимости квазиклассического приближения и теории возмущений приводит к двустороннему ограничению на квантовое число

$$1 \ll n \ll \frac{1}{\sqrt{\epsilon}},$$

что, впрочем, совершенно ясно, поскольку четвертая степень координаты в конце концов начинает доминировать над квадратом при больших значениях x, где, следовательно, возмущение велико.

Киселев-6.2. Квантование в $V = U_0\left(\frac{x^4}{a^4} + \epsilon\frac{x^6}{a^6}\right)$ (????)

Провести квазиклассическое квантование спектра частицы, движущейся в потенциале

$$V = U_0\left(\frac{x^4}{a^4} + \epsilon\frac{x^6}{a^6}\right), \quad U_0 > 0,$$

считая ϵ малым параметром. Провести сравнение с точным спектром при параметре $\zeta := \frac{mU_0}{h^2}a^2 = \frac{1}{6}, \quad \epsilon = 0, 1.$

Solution.

(???? нужно обзор решения дописать!)

Введем безразмерную координату $u = x/a$, в терминах которой стационарное уравнение Шрёдингера для $\psi(u)$ запишется в виде

$$-\frac{h^2}{2ma^2}\psi'' + U_0\left(u^4 + \epsilon u^6\right)\psi = E\psi,$$

или после использования безразмерных параметров глубины потенциальной ямы ζ и энергии $\nu = E/U_0$

$$-\frac{1}{2}\psi'' + \zeta\left(u^4 + \epsilon u^6\right)\psi = \zeta\nu\psi.$$

В задаче без возмущения ($\epsilon \to 0$) правило квантования Бора-Зоммерфельда $\oint p_0(u)\mathrm{d}u = 2\pi\left(n + \frac{1}{2}\right)$ дает

$$\oint p_0(u)\mathrm{d}u = \oint \sqrt{2\left(\zeta\nu - \zeta u^4\right)}\mathrm{d}u = 4\sqrt{2\zeta}\int\limits_0^{\sqrt[4]{\nu}} \mathrm{d}u\sqrt{\nu - u^4},$$

что введением переменной $v = u^4/\nu$ сводится к бета-функции

$$\oint p_0(u)\mathrm{d}u = \sqrt{2\zeta\nu}\sqrt[4]{\nu}\int\limits_0^1 \mathrm{d}v \cdot v^{-\frac{3}{4}}(1-v)^{\frac{1}{2}} = \sqrt{2\zeta}\sqrt[4]{\nu^3}\mathcal{B}\left(\frac{1}{4}, \frac{3}{2}\right) = \sqrt{2\zeta}\sqrt[4]{\nu^3}\frac{\Gamma\left(\frac{1}{4}\right)\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{7}{4}\right)}.$$

Свойства гамма-функции $z\Gamma(z) = \Gamma(z+1), \Gamma(z)\Gamma(1-z) = \pi/\sin(\pi z)$ позволяют записать

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}, \quad \Gamma\left(\frac{7}{4}\right) = \frac{3}{4}\Gamma\left(\frac{3}{4}\right), \quad \Gamma\left(\frac{3}{2}\right) = \frac{1}{2}\Gamma\left(\frac{1}{2}\right), \quad \Gamma\left(\frac{1}{4}\right)\Gamma\left(\frac{3}{4}\right) = \pi\sqrt{2},$$

так что в итоге

$$\oint p_0(u)\mathrm{d}u = \frac{4\pi^2}{3\Gamma^2\left(\frac{3}{4}\right)}\sqrt{\frac{\zeta}{\pi}}v^{\frac{3}{4}}.$$

Введем число

$$g = \frac{3}{2\pi}\Gamma^2\left(\frac{3}{4}\right) \approx 0,717$$

и запишем спектр невозмущенной задачи

$$\nu^{(0)} = \frac{E_n^{(0)}}{U_0} = \left(g\sqrt{\frac{\pi}{\zeta}}\left(n + \frac{1}{2}\right)\right)^{4/3}.$$

Эта формула достаточно точно описывает систему уровней в задаче без возмущения уже при $n > 1$, что видно из рис. 15, где в случае $\zeta = 1/6, \epsilon = 0$ представлена величина $\delta n^{(0)}$, которая определена как приращение к номеру уровня, необходимое пія получения спектра, рассчитанного численно, и задана согласно формуле

$$\nu|_{e=0} = \nu^{(0)} + \frac{\mathrm{d}\nu^{(0)}}{\mathrm{d}n}\delta n^{(0)}$$

Для расчета поправки используем ту же замену переменных в интегралах:

$$\oint \frac{\mathrm{d}u}{p_0(u)} = \frac{\nu^{-\frac{1}{4}}}{\sqrt{2\zeta}}\int\limits_0^1 \mathrm{d}v \cdot v^{-\frac{3}{4}}(1-v)^{-\frac{1}{2}} = \frac{\nu^{-\frac{1}{4}}}{\sqrt{2\zeta}}\frac{\Gamma\left(\frac{1}{4}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{3}{4}\right)}$$

и

$$\oint \frac{\mathrm{d}u}{p_0(u)}u^6 = \frac{\nu^{\frac{5}{4}}}{\sqrt{2\zeta}}\int\limits_0^1 \mathrm{d}v\cdot v^{\frac{3}{4}}(1-v)^{-\frac{1}{2}} = \frac{\nu^{\frac{\pi}{4}}}{\sqrt{2\zeta}}\frac{\Gamma\left(\frac{7}{4}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{9}{4}\right)}$$

откуда по общей формуле

$$\zeta\delta\nu^{(1)} = \zeta\epsilon\left(\oint \frac{\mathrm{d}u}{p_0(u)}u^6\right)/\left(\oint \frac{\mathrm{d}u}{p_0(u)}\right)$$

так что

$$\delta\nu^{(1)} = \epsilon\nu^{\frac{3}{2}}\frac{\Gamma\left(\frac{7}{4}\right)\Gamma\left(\frac{3}{4}\right)}{\Gamma\left(\frac{9}{4}\right)\Gamma\left(\frac{1}{4}\right)} = \epsilon\nu^{\frac{3}{2}}\frac{\frac{3}{4}\Gamma^2\left(\frac{3}{4}\right)}{\frac{5}{4}\frac{1}{4}\Gamma^2\left(\frac{1}{4}\right)} = \frac{8}{15}\epsilon\nu^{\frac{3}{2}}\frac{9\Gamma^4\left(\frac{3}{4}\right)}{4\pi^2}.$$

В итоге

$$\delta\nu^{(1)} = \frac{8}{15}\epsilon g^4\frac{\pi}{\zeta}\left(n+\frac{1}{2}\right)^2.$$

Вычислим эффективный сдвиг номера уровня

$$\delta n = \frac{\delta\nu^{(1)}}{\mathrm{d}\nu^{(0)}/\mathrm{d}n} = \frac{2}{5}\epsilon g^{\frac{8}{3}}\left(\frac{\pi}{\zeta}\right)^{\frac{1}{3}}\left(n+\frac{1}{2}\right)^{\frac{5}{3}} \ll 1.$$

Значит, теория возмущений применима при

$$n \ll \left(\frac{125\zeta}{8g^8\pi\epsilon^3}\right)^{\frac{1}{3}} \approx \frac{7}{3}\left(\frac{\zeta}{\epsilon^3}\right)^{\frac{1}{5}}.$$

Подчеркнем, что прямое сравнение поправки к энергии уровня со значением энергии в невозмущенной задаче привело бы к ошибочной оценке верхней границы области применимости теории возмущений по квантовому числу n, так как необходимо сравнивать поправку с расстоянием между соседними уровнями.

При заданных значениях параметров задачи $\zeta = 1/6, \epsilon = 0,1$ для сравнения приближенных оценок в квазиклассической теории возмущений с точным расположением уровней следует провести численный расчет спектральной задачи. Стандартный прием состоит в том, чтобы построить схему итераций, реализуемую в виде алгоритма. Мы использовали следующий метод: при заданном начальном значении энергии вычислялись точки поворота $a < b$, после чего в качестве начальных

значений задачи Копи бралось квазиклассическое выражение достаточно глубоко в области затухания волновой функции, скажем, правее b; тем самым определялась необходимая для решения уравнения второго порядка первая производная волновой функции в исходной точке $x_0 > b$ с произвольной нормировкой $\psi(x_0)$. Затем вычислялось значение волновой функции в зеркальной точке $\psi(-x_0)$ и определялось значение асимметричности $d = |\psi(x_0)| - |\psi(-x_0)|$. Рис. 15.

Оценка точности квазиклассического приближения по приращению к номеру уровня $\delta n^{(0)}$, которое нужно добавить для согласия с точным численным расчетом энергии связанных состояний, в зависимости от квантового числа n в невозмущенной задаче $\epsilon = 0, \zeta = 1/6$ В изучаемой задаче потенциал - четная функция координаты, так что при верном выборе энергии в спектре уровней асимметричность d должна обращаться в нуль; при этом затухание волновой функции при отрицательных x также гарантировано выбором квазиклассического условия затухания при положительных x. Выбирая пару значений энергии E_1, E_2, легко провести линейную итерацию в точку, где асимметричность должна обратиться в нуль:

$$E_{k+2} = \frac{d_k E_{k+1} - d_{k+1}E_k}{d_k - d_{k+1}}.$$

Этот метод оказывается достаточно точным и быстро сходящимся при малом числе итераций, причем номер уровня контролируется прямым подсчетом числа узлов волновой функции, что легко реализуется в пакете аналитических и численных расчетов и графических построений Mathematica.

Описанная процедура использовалась при численном расчете спектра как невозмущенной задачи, так и при наличии возмущения. Результат сравнения квазиклассических вычислений с точными представлен на рис. 16 в терминах поправки к номеру уровня. Согласно нашему исследованию квазиклассика в совокупности с теорией возмущений может быть применима в ограниченной области значений квантового числа n:

$$1 < n < 7,$$

что и подтверждается данными рис. 16: при малых n, в данном случае для основного состояния, квазиклассика дает плохую оценку и без возмущения, и при его наличии, а при больших n неприменима теория возмущений, так как, во-первых, поправки по сути начинают «перемешивать» соседние уровни, а во-вторых, ведущее приближение оказывается слишком неточным и становится необходимым суммирование поправок высшего порядка, т.е. выход за рамки теории возмущений. Фактически теория возмущений в рамках квазиклассического приближения в этой задаче применима в весьма узкой области квантовых чисел, а именно при $1 < n < 4$.

Киселев-6.3. $e - e^+$ пары в постоянном электрическом поле

В рамках квазиклассического приближения для туннельного эффекта оценить вероятность образования электрон-позитронных пар в постоянном электрическом поле за счет флуктуаций вакуума во внешнем поле.

Solution.

Квантовые флуктуации вакуума, которые приводят к рождению пар частица-античастица, возможны, если энергия флуктуации порядка массы частицы

$$\Delta E \simeq mc^2,$$

а значит, время такой флуктуации согласно соотношению неопределённостей

$$\Delta t \simeq \frac{\hbar}{mc^2}.$$

Если на электрон-позитронную пару в вакуумной флуктуации действует внешнее электрическое поле $\mathcal{E}$, то возникающие силы разводят электрон и позитрон в разные стороны, так что эти виртуальные частицы могут перейти в состолние реальных, наблюдаемых частиц, т.е. может произойти туннельный переход-пробой вакуума. времени равна силе электрического поля;

$$\frac{\Delta p}{\Delta t} = e\mathcal{E} \to \Delta p \simeq \frac{e\hbar\mathcal{E}}{mc^2}.$$

Но флуктуация импульса связана с флуктуацией координаты соотношением неопределённостей

$$\Delta p \cdot \Delta x \simeq \hbar, \quad \Delta x \simeq \frac{mc^2}{e\mathcal{E}}$$

Вероятность туннельного перехода задается квазиклассической формулой

$$w \sim \mathrm{e}^{-2\frac{S}{\hbar}}$$

$$S \simeq \Delta \cdot \Delta x \simeq \hbar \frac{\Delta x}{\lambda_e}$$

где S - действие виртуальной частицы а характерная комптоновская длина волны массивной частицы, согласно критерию применимости квазиклассики, должна быть много меньше ширины потенциального барьера

$$\lambda_e = \frac{\hbar}{mc} \ll \Delta x$$

В итоге, действие

$$S \simeq \frac{m^2c^3}{e\mathcal{E}},$$

а вероятность рождения электрон-позитронной пары в постоянном электрическом поле

$$w \sim \mathrm{e}^{-\mathrm{const}\ \frac{m^2c^3}{k\ell\varepsilon}}.$$

В квантовой теории поля вычисляется и постоянная const $= \pi$, и предэкспоненциальный множитель. Здесь же отметим лишь то, что введение комптоновской длины волны электрона

$$\lambda_e = \frac{\hbar}{mc}$$

позволяет записать аргумент экспоненты в виде фактора

$$\frac{mc^2}{e\mathcal{E}\lambda_e}$$

т.е. он задается отношением массы покоя электрона к работе сил постоянного электрического поля на комптоновской длине волны электрона λ_e Рождение пар из вакуума становится статистически значимым, если значение этого фактора сравнимо с единицей, а значит, когда поле настолько велико, что его напряженность разрывает вакуум на комптоновской длине электрона. Численно это поле чудовищно велико: $\mathcal{E} \sim 10^{14}$ В/.

При осмыслении полученного результата следует обратить внимание на то, что рождение пар частиц в течение бесконечного времени существования поля неминуемо приведет к необходимости учета обратного влияния рождающихся частиц на источники поля (согласно закону сохранения энергии), поэтому в действительности процесс рождения частиц носит существенно нестационарный характер, и при строгом подходе надо рассматривать поля с конечным временем существования.

Киселев-6.4. Рождение фотонов в черной дыре

В рамках квазиклассического приближения для туннельного эффекта определить энергетическую зависимость вероятности рождения пар фотонов в гравитационном поле черной дыры вблизи поверхности Шварцшильда за счет флуктуаций вакуума, если гравитационное ускорение возле сферы Шварцшильда равно $\varkappa c^2$ (для $\varkappa$ вводят термин «поверхностная гравитация»).

Solution.

Предположим, что в вакууме в течение времени Δt имеет место флуктуация: образуется пара фотонов с энергией $E > 0$ и $-E < 0$. На фотон с энергией E и гравитационной массой $m = E/c^2$ действует сила гравитационного поля

$$F = \varkappa c^2 \cdot m = \varkappa E,$$

где, как видим, вместо массы покоя в релятивистском случае стоит энергия частицы. Эта сила направлена к центру черной дыры. На фотон с энергией $-E$ действует такая же по модулю сила, направленная в другую сторону, от центра, так как энергия отрицательна. Таким образом, гравитационные силы растаскивают фотоны из вакуумной флуктуации в разные стороны, так что может иметь место «пробой вакуума», что, естественно, невозможно в отсутствие внешних сил. Поэтому говорят, что под действием гравитационного поля имеет место туннельный переход флуктуации в состояние с реальными фотонами. Сила определяет изменение импульса, так что в конечных приращениях

$$\frac{\Delta p}{\Delta t} \simeq F = \varkappa E,$$

а изменение импульса для фотона связано с энергией флуктуации

$$\Delta p \simeq \frac{E}{c}.$$

Отсюда время флуктуации, в течение которого фотон приобретает энергию E,

$$\Delta t \simeq \frac{1}{\varkappa c}.$$

За это время фотон проходит расстояние

$$\Delta x \simeq c\Delta t \simeq \frac{1}{\varkappa}.$$

Поэтому характерное значение действия S для такой флуктуации

$$S \simeq p \cdot \Delta x \simeq \frac{E}{c} \cdot \frac{1}{x},$$

а вероятность туннельного перехода в квазиклассике

$$w \sim \mathrm{e}^{-2\frac{S}{\hbar}}$$

дает

$$w \sim \mathrm{e}^{-\,\mathrm{const}\,\frac{E}{\hbar\epsilon x}} = \mathrm{e}^{-\beta E}$$

где точное значение постоянной $\mathrm{const} = 2\pi$ было рассчитано Хокингом (Hawking), так что

$$\beta = \frac{2\pi}{\hbar c \varkappa}.$$

В итоге энергетическая зависимость вероятности наблюдения флуктуации повторяет распределение Гиббса для излучения абсолютно черного тела с температурой $kT = 1/\beta$

$$T = \frac{\hbar c}{k} \cdot \frac{\varkappa}{2\pi},$$

где k - постоянная Больцмана и мы выделили фактор из фундаментальных постоянных, который обычно полагают равным единице за счет выбора единиц измерения температуры, длины, времени и энергии.

Значит, гравитационные силы способны приводить к детектированию удаленным наблюдателем фотонов со спектром излучения абсолютно черного тела. При этом, конечно, необходимо, чтобы фотон с отрицательной энергией никогда не попадал в область действия измерительных приборов вне черной дыры. Это действительно возможно при наличии сферы Шварцшильда: тогда при квантовой

флуктуации вблизи этой сферы фотон с положительной энергией достигает удаленного наблюдателя, а фотон с отрицательной энергией падает в черную дыру. В результате энергия черной дыры уменьшается ровно на столько, сколько ее унес с собой фотон к стороннему наблюдателю в измеряемом им спектре излучения. Качественно описанный процесс есть квантовый эффект испарения черных дыр, который носит имя Хокинга.

Отметим, что, подобно предыдущему примеру с рождением пар частица-античастица в электрическом поле, в наших оценочных рассуждениях мы не учитывали нестационарность задачи о возникновении и существовании черной дыры, что в действительности весьма существенно в последовательной теории эффекта Хокинга. Наконец, определим значение поверхностной гравитации из качественных соображений. Фотон не может покинуть черную дыру, так как работа сил гравитации на расстоянии порядка размера черной дыры r_g равна его энергии

$$\varkappa E \cdot r_g \simeq E \to \varkappa \simeq \frac{1}{r_g},$$

так что температура черной дыры обратно пропорциональна размеру черной дыры. Для примера, гравитационный радиус Солнца $\left(M_\odot \approx 2 \cdot 10^{30}\right)$

$$r\odot = \frac{2GM_\odot}{c^2} \approx 3\text{KM},$$

а температура черной дыры с массой Солнца была бы лишь

$$T_\odot \simeq 5 \cdot 10^{-8} K,$$

но масса Солнца недостаточно велика, чтобы гравитационные силы необратимо сжали бы его в черную дыру после исчерпания запасов термоядерного топлива (коллапс Солнца по современным представлениям невозможен).

17.1.15 Problems about variational method (!?)

(потом подумаю про него, пока см. лекции Тонга, если интересно)

17.1.16 Problems about solutions by special functions 1

ПТФ-5.y1

Исследуйте прямоугольную двумерную яму $U(r) = -U_0\theta(a - |r|)$ в обратном пределе глубокой ямы $U_0 \gg \frac{\hbar^2}{Ma^2}$. Оцените N_m – количество связанных состояний в яме для фиксированного орбитального квантового числа $m \in \mathbb{Z}$, а также полное число связанных состояний $N = \sum\limits_m N_m$.

Определите промежуточную асимптотику уровней энергии $E_{n,m}$ (интересны высоколежащие уровни, но не близкие к верху ямы).

Solution.

$$\hat{H}\psi = E\psi$$

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} + U(\vec{r}) = -\frac{\hbar^2}{2m}\Delta - U_0\theta(a - |r|)$$

$$\Delta = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2} = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}$$

$$\psi(r,\varphi) = \psi(r)e^{im\varphi}$$

$$-\frac{\hbar^2}{2M}\left(\psi''(r) + \frac{1}{r}\psi'(r) - \frac{m^2}{r^2}\psi(r)\right) - U_0\theta(a - |r|)\psi(r) = E\psi(r)$$

- Вне ямы $r > a$:

$$-\frac{\hbar^2}{2M}\left(\psi''(r) + \frac{1}{r}\psi'(r) - \frac{m^2}{r^2}\psi(r)\right) = E\psi(r)$$

Пусть $\chi^2 = -\frac{2ME}{\hbar^2}$ и $z = \chi r$, тогда

$$\psi'(r) = \frac{d\psi}{dz}\frac{dz}{dr} = \chi\psi'(z), \quad \psi''(r) = \frac{d\psi'}{dz}\frac{dz}{dr} = \chi^2\psi''(z)$$

$$\psi''(z) + \frac{1}{z}\psi'(z) - \left(1 + \frac{m^2}{z^2}\right)\psi(z) = 0$$

Решение уравнения:

$$\psi(z) = A_1 I_m(z) + A_2 K_m(z)$$

Асимптотика при больших $z \gg 1$:

$$I_m(z) \approx \frac{e^z}{\sqrt{2\pi z}}, \quad K_m(z) \approx \sqrt{\frac{\pi}{2z}}e^{-z}$$

Поскольку волновая функция должна затухать на бесконечности, $A_1 = 0$, $A_2 = A$:

$$\psi(z) = AK_m(z)$$

- Внутри ямы $r < a$:

$$-\frac{\hbar^2}{2M}\left(\psi''(r) + \frac{1}{r}\psi'(r) - \frac{m^2}{r^2}\psi(r)\right) - U_0\psi(r) = E\psi(r)$$

Пусть $k^2 = \frac{2M(U_0+E)}{\hbar^2}$ и $z = kr$, тогда

$$\psi'(r) = \frac{d\psi}{dz}\frac{dz}{dr} = k\psi'(z), \quad \psi''(r) = \frac{d\psi'}{dz}\frac{dz}{dr} = k^2\psi''(z)$$

$$\psi''(z) + \frac{1}{z}\psi'(z) + \left(1 - \frac{m^2}{z^2}\right)\psi(z) = 0$$

Решение уравнения:

$$\psi(z) = B_1 J_m(z) + B_2 Y_m(z)$$

Асимптотика при малых $z \ll 1$:

$$J_m(z) \approx \frac{1}{m!}\left(\frac{z}{2}\right)^m, \quad Y_m(z) \approx \begin{cases} -\frac{(m-1)!}{\pi}\left(\frac{2}{z}\right)^m, & m \neq 0 \\ -\frac{2}{\pi}(\ln\frac{2}{z} - \gamma), & m = 0 \end{cases}$$

Поскольку волновая функция должна быть регулярной в 0, $B_1 = B$, $B_2 = 0$:

$$\psi(z) = BJ_m(z)$$

Сшивка логарифмической производной:

$$\frac{d\ln\psi(a-0)}{dz} = \frac{d\ln\psi(a+0)}{dz} \to \frac{kaJ'_m(ka)}{J_m(ka)} = \frac{\chi aK'_m(\chi a)}{K_m(\chi a)}$$

Рассматривается задача о глубокой яме $U_0 \gg \frac{\hbar^2}{Ma^2}$. поэтому $z \gg 1$. Соответствующие асимптотики при $z \gg 1$:

$$J_m(z) \approx \sqrt{\frac{2}{\pi z}}\cos\left(z - \frac{m\pi}{2} - \frac{\pi}{4}\right), \quad K_m(z) \approx \sqrt{\frac{\pi}{2z}}e^{-z}$$

$$J'_m(z) = -\sqrt{\frac{\pi}{2z^3}}\left(z\sin\left(z - \frac{\pi m}{2} - \frac{\pi}{4}\right) + \frac{1}{2}\cos\left(z - \frac{\pi m}{2} - \frac{\pi}{4}\right)\right), \quad K'_m(z) = -\sqrt{\frac{\pi}{2z^3}}e^{-z}\left(\frac{1}{2} + z\right)$$

Рассмотрим случай $\chi a \gg ka \gg 1$.

$$-ka\frac{1}{ka}\left(ka\tan\left(ka - \frac{\pi m}{2} - \frac{\pi}{4}\right) + \frac{1}{2}\right) = -\chi a\frac{1}{\chi a}\left(\frac{1}{2} + \chi a\right)$$

$$\tan\left(ka - \frac{\pi m}{2} - \frac{\pi}{4}\right) = \frac{\chi}{k} \gg 1$$

$$ka - \frac{\pi m}{2} - \frac{\pi}{4} = \frac{\pi}{2} + \pi n \to ka = \frac{3\pi}{4} + \frac{\pi m}{2} + \pi n$$

$$k^2a^2 = \pi^2\left(\frac{3}{4}+\frac{m}{2}+n\right)^2 = \frac{2Ma^2(U_0-|E_{n.m}|)}{\hbar^2}$$

$$E_{n,m} = U_0 - \frac{\pi^2\hbar^2}{2Ma^2}\left(\frac{3}{4}+\frac{m}{2}+n\right)^2$$

Число решений:

$$N_m = \frac{\sqrt{2Ma^2U_0}}{\pi\hbar} - \frac{m}{2} - \frac{3}{4}$$

$$N_{m_{\max}} = 0 \to m_{\max} = 2\frac{\sqrt{2Ma^2U_0}}{\pi\hbar} - \frac{3}{2}$$

$$N = \sum_{m=0}^{m_{\max}} N_m = \sum_{m=0}^{m_{\max}}\left(\frac{\sqrt{2Ma^2U_0}}{\pi\hbar} - \frac{m}{2} - \frac{3}{4}\right) \approx \frac{m_{\max}(m_{\max}+1)}{2} - \frac{m_{\max}(m_{\max}-1)}{2} = \frac{m_{\max}^2}{4}$$

$$N = \frac{2Ma^2U_0}{\pi^2\hbar^2}$$

ПТФ-5.y2

Определите волновую функцию для движения в трёхмерном Кулоновском потенциале $U(\vec{r}) = -\alpha/r$ частицы с орбитальным квантовым числом L на строго нулевой энергии $E = 0$.
Указание: соответствующее уравнение сводится к уравнению Бесселя.

Solution.

Стационарное уравнение Шрёдингера:

$$\hat{H}\Psi = E\Psi = 0$$

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2M} + U(\vec{r}) = -\frac{\hbar^2}{2M}\Delta - \frac{\alpha}{r}$$

Лапласиан в сферических координатах:

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\varphi^2}$$

Разделим переменные на радиальную и угловую части:

$$\Psi(r,\theta,\varphi) = \psi(r)Y(\theta,\varphi)$$

Уравнение на радиальную часть:

$$-\frac{\hbar^2}{2mr^2}(r^2\psi'(r))' + \left(\frac{\hbar^2L(L+1)}{2mr^2} - \frac{\alpha}{r}\right)\psi(r) = 0$$

$$\psi''(r) + \frac{2}{r}\psi'(r) - \left(\frac{L(L+1)}{r^2} - \frac{2m\alpha}{\hbar r}\right)\psi(r) = 0$$

Сделаем замену $z = 2\sqrt{\frac{2m\alpha r}{\hbar}} \to r = \frac{z^2\hbar}{8m\alpha}$, $u(z) = \psi(r)$:

$$\psi'(r) = \frac{d\psi}{dr} = \frac{dz}{dr}\frac{du}{dz} = \sqrt{\frac{2m\alpha}{\hbar r}}u'(z) = \frac{4m\alpha}{\hbar z}u'(z)$$

$$\psi''(r) = \frac{d^2\psi}{dr^2} = \frac{4m\alpha}{\hbar z}\frac{d}{dz}\left(\frac{4m\alpha}{\hbar z}u'(z)\right) = \frac{16m^2\alpha^2}{\hbar^2z^3}u'(z) + \frac{16m^2\alpha^2}{\hbar^2z^2}u''(z)$$

$$\frac{16m^2\alpha^2}{\hbar^2z^2}u''(z) + \frac{48m^2\alpha^2}{\hbar^2z^3}u'(z) + \frac{16m^2\alpha^2}{\hbar^2z^2}\left(1 - \frac{4L(L+1)}{z^2}\right)u(z) = 0$$

$$z^2u''(z) + 3zu'(z) + (z^2 - 4L(L+1))u(z) = 0$$

Сделаем замену $v(z) = zu(z) \to u(z) = \frac{v(z)}{z}$:

$$u'(z) = \frac{v'(z)}{z} - \frac{v(z)}{z^2}, \quad u''(z) = \frac{v''(z)}{z} - \frac{2v'(z)}{z^2} + \frac{2v(z)}{z^3}$$

$$zv''(z) - 2v'(z) + \frac{2v(z)}{z} + 3v'(z) - \frac{3v(z)}{z} + zv(z) - \frac{4L(L+1)}{z}v(z) = 0$$

$$v''(z) + \frac{1}{z}v'(z) + \left(1 - \frac{(2L+1)^2}{z^2}\right)v(z) = 0$$

Получилось уравнение Бесселя с $m = 2L + 1$. Его решение:

$$v(z) = A_1 J_{2L+1}(z) + A_2 Y_{2L+1}(z)$$

Вернёмся к замене:

$$\psi(r) = \frac{1}{2}\sqrt{\frac{\hbar}{2m\alpha r}}\left(A_1 J_{2L+1}\left(2\sqrt{\frac{2m\alpha r}{\hbar}}\right) + A_2 Y_{2L+1}\left(2\sqrt{\frac{2m\alpha r}{\hbar}}\right)\right)$$

ПТФ-5.з1

Рассмотрите трёхмерную частицу массы m, движущуюся в трёхмерной шаровой полости радиуса a с бесконечными стенками:

$$U(\vec{r}) = \begin{cases} 0, & |\vec{r}| < a \\ \infty, & |\vec{r}| > a \end{cases}$$

Каким уравнением определяются уровни энергии с фиксированным орбитальным моментом L? Решите уравнение точно для $L = 0$, а также приближённо для высоколежащих уровней энергии при $L \geq 1$.

Указание: свободное движение в трёхмерном пространстве также сводится к функциям Бесселя, но с полуцелым индексом $J_{n+1/2}(z)$ (которые, в действительности, специальными функциями не являются, а имеют явное представление через обычные тригонометрические функции).

Solution.

При $r > a$:

$$\psi(r) = 0$$

Стационарное уравнение Шрёдингера при $r < a$ для радиальной части:

$$\psi''(r) + \frac{2}{r}\psi'(r) + \left(\frac{2mE}{\hbar^2} - \frac{L(L+1)}{r^2}\right)\psi(r) = 0$$

Введём замену $\psi(r) = \frac{u(r)}{\sqrt{r}}$.

$$\psi'(r) = \frac{u'(r)}{\sqrt{r}} - \frac{u(r)}{2r^{\frac{3}{2}}}, \quad \psi''(r) = \frac{u''(r)}{\sqrt{r}} - \frac{u'(r)}{r^{\frac{3}{2}}} + \frac{3u(r)}{4r^{\frac{5}{2}}}$$

$$\frac{u''(r)}{\sqrt{r}} - \frac{u'(r)}{r^{\frac{3}{2}}} + \frac{3u(r)}{4r^{\frac{5}{2}}} + \frac{2u'(r)}{r^{\frac{3}{2}}} - \frac{u(r)}{r^{\frac{5}{2}}} + \left(\frac{2mE}{\hbar^2} - \frac{L(L+1)}{r^2}\right)\frac{u(r)}{\sqrt{r}} = 0$$

$$u''(r) + \frac{u'(r)}{r} + \left(\frac{2mE}{\hbar^2} - \frac{L(L+1)}{r^2} - \frac{1}{4}\right)u(r) = 0$$

$$u''(r) + \frac{u'(r)}{r} + \left(\frac{2mE}{\hbar^2} - \frac{(L+\frac{1}{2})^2}{r^2}\right)u(r) = 0$$

$$u(r) = B_1 J_{L+\frac{1}{2}}\left(\frac{\sqrt{2mE}}{\hbar}r\right) + B_2 Y_{L+\frac{1}{2}}\left(\frac{\sqrt{2mE}}{\hbar}\right)$$

Вернёмся к замене:

$$\psi(r) = \frac{B_1}{\sqrt{r}} J_{L+\frac{1}{2}}\left(\frac{\sqrt{2mE}}{\hbar}r\right) + \frac{B_2}{\sqrt{r}} Y_{L+\frac{1}{2}}\left(\frac{\sqrt{2mE}}{\hbar}r\right)$$

Поскольку функция Неймана сингулярна в 0, то $B_2 = 0$. Сшивка при $r = a$:

$$J_{L+\frac{1}{2}}\left(\frac{\sqrt{2mE}a}{\hbar}\right) = 0$$

- Случай $L = 0$.

$$\sqrt{\frac{2\hbar}{\pi a\sqrt{2mE}}}\sin\left(\frac{\sqrt{2mE}a}{\hbar}\right) = 0 \to \frac{\sqrt{2mE}a}{\hbar} = \pi n$$

$$E_n = \frac{\pi^2\hbar^2 n^2}{2ma^2}$$

- Случай $L \geq 1$. Для высоколежащих уровней $\frac{\sqrt{2mE}a}{\hbar} \gg 1$. Асимптотика функции Бесселя при $z \gg 1$:

$$J_m(z) \approx \sqrt{\frac{2}{\pi z}}\cos\left(z - \frac{m\pi}{2} - \frac{\pi}{4}\right)$$

$$\frac{\sqrt{2\hbar}}{\sqrt{\pi a\sqrt{2mE}}}\cos\left(\frac{\sqrt{2mE}a}{\hbar} - \frac{(L+\frac{1}{2})\pi}{2} - \frac{\pi}{4}\right) = 0$$

$$\sin\left(\frac{\sqrt{2mE}a}{\hbar} - \frac{\pi L}{2}\right) = 0$$

$$\frac{\sqrt{2mE}a}{\hbar} - \frac{\pi L}{2} = \pi n$$

$$E_n = \frac{\pi^2\hbar^2(2n+L)^2}{8ma^2}$$

ПТФ-5.з2. Ступенька (40 б).

Определите коэффициенты прохождения и отражения от потенциала $U(x) = \frac{1}{2}U_0\tanh\frac{x}{a}$. Указание: при помощи замены $\xi = -e^{-2x/a}$ задача приводится к гипергеометрической функции ${}_2F_1$.

Solution.

Стационарное уравнение Шрёдингера:

$$-\frac{\hbar^2}{2m}\psi''(x) + \left(\frac{1}{2}U_0\tanh\frac{x}{a} - E\right)\psi(x) = 0$$

Пусть $\xi = -e^{-\frac{2x}{a}}$, тогда $x = -\frac{a}{2}\ln(-\xi)$.

$$\text{th}\,\frac{x}{a} = \frac{1+\xi}{1-\xi}$$

$$\psi'(x) = -\frac{2}{a}\xi\psi'(\xi), \quad \psi''(x) = \frac{4\xi}{a^2}\psi'(\xi) + \frac{4\xi^2}{a^2}\psi''(\xi)$$

Пусть $k^2 = \frac{ma^2}{4\hbar^2}U_0$, $\kappa^2 = \frac{ma^2}{2\hbar^2}E$.

$$\xi\frac{\partial\psi}{\partial\xi} + \xi^2\frac{\partial^2\psi}{\partial\xi^2} + k^2\frac{\xi+1}{\xi-1}\psi + \kappa^2\psi = 0$$

$$\psi(\xi) = \Psi(\xi)\xi^{\sqrt{k^2-\chi^2}}$$

$$\xi(1-\xi)\Psi''(\xi) - (2\sqrt{k^2-\kappa^2}+1)(\xi-1)\Psi'(\xi) - 2k^2\Psi(\xi) = 0$$

$$\Psi(\xi) = C_1\xi^{\sqrt{k^2-\kappa^2}}{}_2F_1(\sqrt{-k^2-\kappa^2}+\sqrt{k^2-\kappa^2}, -\sqrt{-k^2-\kappa^2}+\sqrt{k^2-\kappa^2}, 1+2\sqrt{k^2-\chi^2}, \xi) +$$
$$+ C_2\xi^{-\sqrt{k^2-\kappa^2}}{}_2F_1(-\sqrt{k^2-\kappa^2}-\sqrt{-k^2-\kappa^2}, -\sqrt{k^2-\kappa^2}+\sqrt{-k^2-\kappa^2}, 1-2\sqrt{k^2-\chi^2}, \xi)$$

Рассмотрим 2 базисное решение:

$$\psi(\xi) = \xi^{-i\sqrt{\kappa^2-k^2}}{}_2F_1(-\sqrt{k^2-\kappa^2}-\sqrt{-k^2-\kappa^2}, -\sqrt{k^2-\kappa^2}+\sqrt{-k^2-\kappa^2}, 1-2\sqrt{k^2-\chi^2}, \xi)$$

При $x \to \infty$

$$ {}_2F_1(..., e^{-\frac{2x}{a}}) \sim 1$$

$$\psi(x) = (-1)^{i\sqrt{k^2+\kappa^2}} e^{-i\frac{2x}{a}\sqrt{k^2+\kappa^2}} = e^{\pi\sqrt{\kappa^2-k^2}} e^{i\frac{2x}{a}\sqrt{\kappa^2-k^2}}$$

При $x \to -\infty$

$$\frac{\sin(\pi(b-a))}{\pi}{}_2F_1(a,b,c,\xi) = \frac{(-\xi)^a}{\Gamma(b)\Gamma(c-a)}{}_2F_1(a, a-c+1, a-b+1, \frac{1}{\xi}) - \\ - \frac{(-\xi)^{-b}}{\Gamma(a)\Gamma(c-b)}{}_2F_1(b, b-c+1, b-a+1, \frac{1}{\xi})$$

$$ {}_2F_1(a,b,c,\frac{1}{\xi}) \sim 1$$

$$\Psi(\xi) = -\frac{\pi}{i\sinh(\pi\sqrt{k^2+\kappa^2})} e^{\pi\sqrt{\kappa^2-k^2}} \left(\frac{e^{-i\frac{2x}{a}\sqrt{k^2+\kappa^2}}}{(i\sqrt{\kappa^2-k^2}-i\sqrt{\kappa^2+k^2})\Gamma^2(i\sqrt{\kappa^2-k^2}-i\sqrt{\kappa^2+k^2})} - \right. \\ \left. - \frac{e^{i\frac{2x}{a}\sqrt{k^2+\kappa^2}}}{(i\sqrt{\kappa^2-k^2}+i\sqrt{\kappa^2+k^2})\Gamma^2(i\sqrt{\kappa^2-k^2}+i\sqrt{\kappa^2+k^2})} \right)$$

$$r = \frac{\pi i}{\sinh \pi\sqrt{\kappa^2+k^2}} (i\sqrt{\kappa^2-k^2}+i\sqrt{\kappa^2+k^2})\Gamma^2(i\sqrt{\kappa^2-k^2}+i\sqrt{\kappa^2+k^2})$$

$$t = \frac{\pi i}{\sinh \pi\sqrt{\kappa^2+k^2}} (i\sqrt{\kappa^2-k^2}-i\sqrt{\kappa^2+k^2})\Gamma^2(i\sqrt{\kappa^2-k^2}-i\sqrt{\kappa^2+k^2})$$

Определим коэффициенты отражения и прохождения. Упростим r и t и получим:

$$R = |r|^2 = \frac{\sinh^2(\pi(\sqrt{\kappa^2-k^2}-\sqrt{\kappa^2+k^2}))}{\sinh^2(\pi(\sqrt{\kappa^2-k^2}+\sqrt{\kappa^2+k^2}))}$$

$$T = \frac{\sqrt{\kappa^2+k^2}}{\sqrt{\kappa^2-k^2}}|t|^2 = \frac{\sinh(2\pi(\sqrt{\kappa^2-k^2}))\sinh(2\pi\sqrt{\kappa^2+k^2}))}{\sinh^2(\pi(\sqrt{\kappa^2-k^2}+\sqrt{\kappa^2+k^2}))}$$

ПТФ-6.у1. Функция Эйри

Используя асимптотики функций Эйри для инфинитного движения (без бесконечной стенки), отнормируйте их на дельта-функцию от энергии, а также убедитесь в соотношении полноты. А именно, выпишите волновые функции, удовлетворяющие следующему условию:

$$\int dx \psi^*_E(x)\psi_{E'}(x) = \delta(E-E')$$

и убедитесь, что для них выполняется соотношение

$$\int dE \psi^*_E(x')\psi_E(x) = \delta(x-x')$$

Solution.

$$-\frac{\hbar^2}{2m}\psi''(x) + Fx\psi(x) = E\psi(x)$$

$$z = \frac{x - E/F}{(\hbar^2/2mF)^{\frac{1}{3}}}$$

$$\psi''(z) - z\psi(z) = 0$$

Общее решение – произвольная линейная комбинация функций Эйри первого и второго рода:

$$\psi(z) = C_1 \mathrm{Ai}(z) + C_2 \mathrm{Bi}(z)$$

Асимптотики функции Эйри:

$$\mathrm{Ai}(z) \approx \begin{cases} \frac{1}{2\sqrt{\pi} z^{\frac{1}{4}}} \exp\left(-\frac{2}{3} z^{\frac{3}{2}}\right), & z \to \infty \\ \frac{1}{\sqrt{\pi}(-z)^{\frac{1}{4}}} \sin\left(\frac{2}{3}(-z)^{\frac{3}{2}} + \frac{\pi}{4}\right), & z \to -\infty \end{cases}$$

$$\frac{1}{\sqrt{\pi}(-z)^{\frac{1}{4}}} \sin\left(\frac{2}{3}(-z)^{\frac{3}{2}} + \frac{\pi}{4}\right) = \frac{1}{2\sqrt{\pi}(-z)^{\frac{1}{4}}} \left(e^{i\left(\frac{2}{3}(-z)^{\frac{3}{2}} - \frac{\pi}{4}\right)} + e^{-i\left(\frac{2}{3}(-z)^{\frac{3}{2}} + \frac{3\pi}{4}\right)}\right)$$

$$\psi_E(x) = C\mathrm{Ai}(z)$$

$$\int dx \psi_E^*(x)\psi_{E'}(x) =$$

$$= \frac{C^2}{4\pi(zz')^{\frac{1}{4}}} \int\limits_{-\infty}^{0} dx \left(e^{-i\left(\frac{2}{3}(-z)^{\frac{3}{2}} - \frac{\pi}{4}\right)} + e^{i\left(\frac{2}{3}(-z)^{\frac{3}{2}} + \frac{3\pi}{4}\right)}\right)\left(e^{i\left(\frac{2}{3}(-z')^{\frac{3}{2}} - \frac{\pi}{4}\right)} + e^{-i\left(\frac{2}{3}(-z')^{\frac{3}{2}} + \frac{3\pi}{4}\right)}\right) +$$

$$+ \frac{C^2}{4\pi(zz')^{\frac{1}{4}}} \int\limits_{0}^{\infty} dx \left(e^{-i\left(\frac{2}{3}(-z)^{\frac{3}{2}} - \frac{\pi}{4}\right)} + e^{i\left(\frac{2}{3}(-z)^{\frac{3}{2}} + \frac{3\pi}{4}\right)}\right)\left(e^{i\left(\frac{2}{3}(-z')^{\frac{3}{2}} - \frac{\pi}{4}\right)} + e^{-i\left(\frac{2}{3}(-z')^{\frac{3}{2}} + \frac{3\pi}{4}\right)}\right) + \mathrm{reg.} =$$

$$= \frac{C^2}{4\pi(zz')^{\frac{1}{4}}} \int\limits_{-\infty}^{0} dx \left(e^{\frac{2i}{3}\left((-z')^{\frac{3}{2}} - (-z)^{\frac{3}{2}}\right)} + e^{-\frac{2i}{3}\left((-z')^{\frac{3}{2}} - (-z)^{\frac{3}{2}}\right)}\right) + \mathrm{reg.}$$

$$\Delta z = z - z' = \frac{\Delta E}{F}\left(\frac{2mF}{\hbar^2}\right)^{\frac{1}{3}}$$

$$\int dx \psi_E^*(x)\psi_{E'}(x) = \frac{C^2}{4\pi z^{\frac{1}{2}}}\left(\frac{\hbar^2}{2mF}\right)^{\frac{1}{3}} \int\limits_{-\infty}^{0} dz (e^{-\frac{2}{3}i(-z)^{\frac{3}{2}}\frac{3\Delta z}{2z}} + e^{\frac{2}{3}i(-z)^{\frac{3}{2}}\frac{3\Delta z}{2z}}) =$$

$$= \left(\frac{\hbar^2}{2mF}\right)^{\frac{1}{3}} \frac{C^2}{2\pi} \int\limits_{-\infty}^{\infty} d(\sqrt{z}) e^{-i\Delta z\sqrt{z}} = C^2 \left(\frac{\hbar^2\sqrt{F}}{2m}\right)^{\frac{2}{3}} \delta(E' - E) = \delta(E' - E)$$

$$C = \left(\frac{2m}{\hbar^2\sqrt{F}}\right)^{\frac{1}{3}}$$

$$\psi_E(x) = \left(\frac{2m}{\hbar^2\sqrt{F}}\right)^{\frac{1}{3}} \mathrm{Ai}\left(\frac{x - E/F}{(\hbar^2/2mF)^{\frac{1}{3}}}\right)$$

$$\int dE \psi_E^*(x')\psi_E(x) = \frac{C^2}{4\pi} \int\limits_{-\infty}^{0} dE \left(e^{\frac{2i}{3}\left((-z')^{\frac{3}{2}} - (-z)^{\frac{3}{2}}\right)} + e^{-\frac{2i}{3}\left((-z')^{\frac{3}{2}} - (-z)^{\frac{3}{2}}\right)}\right) + \mathrm{reg.} =$$

$$= -\frac{FC^2}{4\pi}\left(\frac{\hbar^2}{2mF}\right)^{\frac{1}{3}} \int\limits_{-\infty}^{0} dz \frac{e^{iz^{\frac{1}{2}}\Delta z} + e^{-iz^{\frac{1}{2}}\Delta z}}{z^{\frac{1}{2}}} = FC^2\left(\frac{\hbar^2}{2mF}\right)^{\frac{2}{3}} \delta(x - x') = \delta(x - x')$$

$$\int dE \psi_E^*(x')\psi_E(x) = \delta(x - x')$$

ПТФ-6.з3. Hydrogen atom in 2D

Определите уровни энергии и кратности их вырождения, а также стационарные волновые функции для двумерной частицы, движущейся в притягивающем потенциале $U(\vec{r}) = -\frac{e^2}{r}$.

Указание: задача приводится к вырожденной гипергеометрической функции ${}_1F_1$.

Solution.

Стационарное уравнение Шрёдингера:

$$-\frac{\hbar^2}{2M}\Delta\psi - \frac{e^2}{r}\psi = E\psi$$

$$-\frac{\hbar^2}{2M}\left(\frac{\partial^2\psi}{\partial r^2} + \frac{1}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\varphi^2}\right) - \frac{e^2}{r}\psi = E\psi$$

Разделим переменные:

$$\psi(r,\varphi) = R(r)e^{im\varphi}$$

$\kappa^2 := -\frac{2mE}{\hbar^2}$.

$$\frac{\partial^2 R}{\partial r^2} + \frac{1}{r}\frac{\partial R}{\partial r} - \left(\frac{2Me^2}{\hbar^2 r} + \kappa^2 + \frac{m^2}{r^2}\right)R = 0$$

$x := \kappa r$,

$$R'' + \frac{R'}{x} - \left(1 + \frac{2Me^2}{\hbar^2\kappa x} + \frac{m^2}{x^2}\right)R = 0$$

$R := x^m f$:

$$R' = mx^{m-1}f + x^m f', \quad R'' = m(m-1)x^{m-2}f + 2mx^{m-1}f' + x^m f''$$

$$xf'' + (2m+1)f' - \left(x + \frac{2Me^2}{\hbar^2\kappa}\right)f = 0$$

$$x \to \infty : f'' - f = 0 \to f \sim e^{-x}$$

$f(x) := e^{-x}\chi(x)$.

$$f'(x) = -e^{-x}\chi + e^{-x}\chi', \quad f''(x) = e^{-x}\chi - 2e^{-x}\chi' + e^{-x}\chi''$$

$$x\chi'' + (2m+1-2x)\chi' - \left(2m+1+\frac{2Me^2}{\hbar^2\kappa}\right)\chi = 0$$

$$\chi(x) = C_1 F_1\left(m + \frac{1}{2} - \frac{Me^2}{\hbar^2\kappa}, 2m+1, 2x\right)$$

Второе линейно независимое решение сингулярно в 0.

$$m + \frac{1}{2} - \frac{Me^2}{\hbar^2\kappa} = -n$$

$$E_{n,m} = -\frac{\hbar^2}{2M}\chi^2 = -\frac{Me^2}{2\hbar^2\left(|m| + n + \frac{1}{2}\right)^2}$$

Пусть $N = |m| + n$, тогда кратность вырождения:

$$K = 2N - 1$$

$$\psi(r,\varphi) = Ce^{im\varphi}\left(\frac{\sqrt{-2mE}}{\hbar}r\right)^{|m|} e^{-\frac{\sqrt{-2mE}}{\hbar}r}\,{}_1F_1\left(-n, 2m+1, 2\frac{\sqrt{-2mE}}{\hbar}r\right)$$

ГК-1.10. Волновые функции и спектр в поле $V(x) = V_0\left(\frac{a}{x} - \frac{x}{a}\right)^2$

Найти волновые функции и уровни энергии частицы в поле вида $V(x) = V_0\left(\frac{a}{x} - \frac{x}{a}\right)^2$ $(x > 0)$ (см. рис. 2) и показать, что энергетический спектр совпадает со спектром осциллятора

ГК-1.11. Спектр в $V = -\frac{V_0}{\mathrm{ch}^2\frac{x}{a}}$

Определить уровни энергии для частицы, находящейся в потенциальном поле $V = -\frac{V_0}{\mathrm{ch}^2\frac{x}{a}}$

Solution.

Типично задача решается переходом к гипергеометрической функцией подстановкой, а затем заменой координат.

(еще раз перепишу компактнее потом решение, а также добавлю вычисления. укажу в теории обязательно эти ходы!!!)

Решаем уравнение Шредингера

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2}-\left(E+\frac{V_0}{\operatorname{ch}^2\frac{x}{a}}\right)\psi=0$$

с помощью подстановки $\psi=\left(\operatorname{ch}\frac{x}{a}\right)^{-2\lambda}u,\quad \lambda=\frac{1}{4}\left(\sqrt{\frac{8\mu V_0a^2}{\hbar^2}+1}-1\right)$

(тут пара промежуточных вычислений)

Уравнение для u примет следующий вид:

$$\frac{d^2u}{dx^2}-\frac{4\lambda}{a}\operatorname{th}\frac{x}{a}\frac{du}{dx}+\frac{4}{a^2}\left(\lambda^2-\varkappa^2\right)u=0,$$

где $\varkappa=\sqrt{-\frac{\mu Ea^2}{2\hbar^2}}$. (рассматриваем дискретный спектр $E<0$). Далее, введем

$$z=-\operatorname{sh}^2\frac{x}{a},$$

и это уравнение сведем к гипергеометрическому уравнению

$$z(1-z)\frac{d^2u}{dz^2}+\left[\frac{1}{2}-(1-2\lambda)z\right]\frac{du}{dz}-\left(\lambda^2-\varkappa^2\right)u=0.$$

Параметры α,β,γ, входящие в гипергеометрическое уравнение общего вида

$$z(1-z)\frac{d^2u}{dz^2}+[\gamma-(\alpha+\beta+1)z]\frac{du}{dz}-\alpha\beta u=0$$

имеют в нашем случае следующие значения:

$$\gamma=\frac{1}{2},\quad \alpha=\varkappa-\lambda,\quad \beta=-\varkappa-\lambda.$$

Два решения, которые дают соответственно четные и нечетные волновые функции ψ; имеют вид

$$u_1=F\left(-\lambda+x,-\lambda-x,\frac{1}{2};z\right)$$
$$u_2=\sqrt{z}F\left(-\lambda+x+\frac{1}{2},-\lambda-x+\frac{1}{2},\frac{3}{2};z\right)$$

Эти решения приводят к ограниченным значениям волновых функций при $x=0(z=0)$.

Для того чтобы волновая функция

$$\zeta=\left(\operatorname{ch}\frac{x}{a}\right)^{-2\lambda}u$$

обращалась в нуль при $x\to\pm\infty(z\to-\infty)$, гипергеометрические функции в выражениях (2) и (3) должны сводиться к полиномам. это условие означает, например, для u_1, что либо $\lambda-x$, либо $\lambda+x$ являются целыми неотрицательными числами. Однако второй случай должен быть отброшен, так как при этом волновая функция при $x\to\pm$ $\pm$ экспоненциально возрастает. Итак, получаем $\lambda-\%=k(k=0,\,1,2,...)$ и уровни энергии

$$E_k=-\frac{t^2}{2\mu\cdot a^2}\left[\frac{1}{2}\sqrt{\frac{8\mu V_0a^2}{\hbar^2}+1}-2k-\frac{1}{2}\right]^2.$$

Аналогично этому для выражения (3) находим, что условие конечности волновой функции при $x\to\pm\infty$ выполняется, если

$$\lambda-x-\frac{1}{2}=l\quad(l=0,1,2,...)$$

откуда

$$E_l=-\frac{\hbar^2}{2\mu a^2}\left[\frac{1}{2}\sqrt{\frac{8\mu V_0a^2}{\hbar^2}+1}-(2l+1)-\frac{1}{2}\right]^2.$$

Объединяя эти выражения, находим:

$$E_n = -\frac{\hbar^2}{2\mu a^2}\left[\frac{1}{2}\sqrt{\frac{8\mu V_0 a^2}{\hbar^2}+1}-\left(n+\frac{1}{2}\right)\right]^2$$

Число дискретных уровней равно наибольшему целому числу N, удовлетворяющему неравенству

$$N < \frac{1}{2}\sqrt{\frac{8\mu V_0 a^2}{\hbar^2}+1}-\frac{1}{2}.$$

Отметим, что полученный спектр энергий совпадает при соответствующем выборе параметров со спектром для потенциала Морза (???).

ПТФ.?. Рассеяние в $V = -\frac{V_0}{\mathrm{ch}^2\frac{x}{a}}$

Определить (???)

Solution.

Решим задачу рассеяния для $E > 0$ в потенциале вида $U(x) = -U_0/\,\mathrm{ch}^2(x/a)$.

Удобно воспользоваться параметризацией $E = k^2/2m$, и решение можно получить из выписанного выше простой заменой $\kappa a = -ika$:

$$\psi(z) = (z(1-z))^{-ika/2}\cdot{}_2F_1(-ika-s,-ika+s+1;-ika+1;z),\quad z=\frac{1}{2}(1-\tanh(x/a))$$

Мы получили какое-то решение непрерывного спектра; однако, ещё не факт что оно соответствует задаче рассеяния.

Тем не менее, даже если и не соответствует - задачу рассеяния мы всё равно сможем построить, выбрав линейную комбинацию с комплексно сопряжённым решением (которое является вторым линейно-независимым).

Чтобы это понять, нам необходимо найти асимптотическое поведение этого решения на бесконечности.

При $x \to +\infty \to y = \tanh\frac{x}{a} \approx 1-2e^{-2x/a} \to z \approx e^{-2x/a} \to 0$, гипергеометрическая функция ${}_2F_1(...,z) \approx 1$. Поэтому:

$$\psi(x \gg a) \approx e^{ikx}$$

Поскольку $z \approx 1$, то в правой части тождества непосредственно гипергеометрические функции раскладываются как ${}_2F_1(...;1-z) \approx 1$, и основная асимптотика определяется выражениями с Гамма-функциями и $(1-z)^{c-a-b} = (1-z)^{ika} \approx e^{2ikx}$ Вспоминая также о префакторе $(z(1-z))^{-ika/2} \approx e^{-ikx}$, мы немедленно получаем асимптотику волновой функции при $x \to -\infty$, которая, следуя общей логике задачи рассеяния, содержит падающую и отражённую волну:

$$\psi(x\to-\infty) = \frac{\Gamma(-ika+1)\Gamma(-ika)}{\Gamma(-ika-s)\Gamma(-ika+s+1)}e^{ikx} + \frac{\Gamma(-ika+1)\Gamma(-ika)}{\Gamma(s+1)\Gamma(-s)}e^{-ikx}$$

Обычно в задаче рассеяния коэффициент при падающей волне e^{ikx} берётся равным единице; тогда остальные коэффициенты отвечают амплитуде отражения и прохождения.

У нас нормировка чуть другая, и амплитуды даются отношением коэффициентов:

$$t = \frac{\Gamma(-ika-s)\Gamma(-ika+s+1)}{\Gamma(-ika+1)\Gamma(-ika)},\quad r = \frac{\Gamma(-ika-s)\Gamma(-ika+s+1)}{\Gamma(s+1)\Gamma(-s)}$$

Это - окончательный ответ, но его можно упросить, используя $\Gamma(z)^* = \Gamma(z^*), \Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin\pi z}, \Gamma(z+1) = z\Gamma(z)$, получим:

$$T = |t|^2 = \frac{\mathrm{sh}^2(\pi ka)}{\mathrm{sh}^2(\pi ka)+\sin^2(\pi s)},\quad R = |r|^2 = \frac{\sin^2(\pi s)}{\mathrm{sh}^2(\pi ka)+\sin^2(\pi s)}$$

Такой ответ уже нам симпатичен.

(???? дальше комментарии???))

Можно проверить, насколько полученный ответ физичен. Во-первых, разумеется, для него выполняется общее соотношение, накладываемое унитарностью квантовой механики $R+T=1$; при большой энергии $ka \gg 1$, коэффициент отражения уменьшается, что разумно -ведь движение с большой

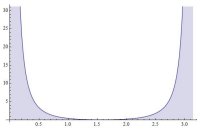
энергией квазиклассично, а в классической механике частица, пролетающая над ямой (или горбом!) совершенно не рассеивается.

Любопытно также, про при целом $s \in \mathbb{Z}$, коэффициент отражения обращается в ноль (на уровне амплитуды отражения это соответствует тому, что у аналитической функции $\Gamma(z)$ имеются полюса первого порядка при $z = -s$) -имеется резонансное безотражательное рассеяние на всех эжергиях! Выше мы получили, что целое s также соответствует ситуации, когда в яме зарождается очередное связанное состояние.

*) Настоящая задача тесно связана со следующей задачей классической механики: дан период колебаний как функция энергии частицы, требуется найти потенциальную энергию (см. Ландау и Пятигорский, «Механика", Гостехиздат, 1940, где даио решение этой задачи)

ГК-1.12. Спектр и волновые функции в $V = V_0 \operatorname{ctg}^2 \frac{\pi}{a}$

Определить энергетические уровни и волновые функции частицы в поле $V = V_0 \operatorname{ctg}^2 \frac{\pi}{a} x (0 < x < a)$



Произвести нормировку волновой функции основного состояния, рассмотреть предельные случаи малых и больших значений V_0.

Solution.

Делаем замену, приходим к гипергеометрической функции, уровни энергии из ее нулей.
(??? как догадаться про это и про конкретные преобразования?? в 1ю позже допишу)

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2} - \left(E - V_0 \operatorname{ctg}^2 \frac{\pi}{a}x\right)\psi = 0$$

$$\psi \equiv \left(\sin \frac{\pi}{a}x\right)^{-2\lambda} u$$

$$\lambda := \frac{1}{4}\left(\sqrt{\frac{8\mu V_0 a^2}{\pi^2\hbar^2} + 1} - 1\right),$$

$$\nu := \sqrt{\frac{\mu a^2}{2\hbar^2\pi^2}(E + V_0)}$$

(тут вставлю эти вычисления)

$$\frac{d^2u}{dx^2} - 4\frac{\pi}{a}\lambda \operatorname{ctg}\frac{\pi x}{a}\frac{du}{dx} + \frac{4\pi^2}{a^2}\left(\nu^2 - \lambda^2\right)u = 0.$$

$$z := \cos^2 \frac{\pi x}{a}$$

получаем гипергеометрическое уравнение:

$$z(1-z)\frac{d^2u}{dz^2} + \left[\frac{1}{2} - (1-2\lambda)z\right]\frac{du}{dz} + \left(\nu^2 - \lambda^2\right)u = 0.$$

Сравнивая с общим его видом $z(1-z)\frac{d^2u}{dz^2} + [\gamma - (\alpha+\beta+1)z]\frac{du}{dz} - \alpha\beta u = 0$, находим параметры:

$$\gamma = \frac{1}{2}, \quad \alpha = -\nu - \lambda, \quad \beta = \nu - \lambda.$$

Полученное уравнение имеет два решения. Одно из этих решений отлично от нуля и конечно при $z = 0$ (этому значению соответствует $x = a/2$)

$$u_1 = F\left(-\nu - \lambda, \nu - \lambda, \frac{1}{2}; z\right).$$

Другое решение

$$u_2 = \sqrt{z}F\left(-\nu - \lambda + \frac{1}{2}, v - \lambda + \frac{1}{2}, \frac{3}{2}; z\right)$$

обращается в нуль при $z=0\left(x=\frac{a}{2}\right)$. Чтобы определить поведение решений при $z=1$ (это значение соответствует $x=0, x=a$), воспользуемся $F(\alpha,\beta,\gamma;z)=(1-z)^{-\alpha}F\left(\alpha,\gamma-\beta,\gamma;\frac{z}{z-1}\right)$:

$$u_1=(1-z)^{\nu+\lambda}F\left(-\nu-\lambda,-\nu+\lambda+\frac{1}{2},\frac{1}{2};\frac{z}{z-1}\right)$$
$$u_2=\sqrt{z}(1-z)^{v+\lambda-\frac{1}{2}}F\left(-\nu-\lambda+\frac{1}{2},-v+\lambda+1,\frac{3}{2};\frac{z}{z-1}\right)$$

Для того чтобы выполнялось условие обращения в нуль волновой функции ψ при $x=0$ и $x=a$, необходимо, чтобы ряды по степеням $\frac{z}{z-1}$ содержали конечное число членов.

Гипергеометрический ряд для u_1 обрывается, если либо $\nu+\lambda$ - целое положительное число или нуль, либо $\nu-\lambda-\frac{1}{2}$ - целое положительное число или нуль. Однако условию $\psi=0$ при $x=0, x=a$ удовлетворяет только второй случай (??? почему?? видимо, в теории это доказано)

$$\nu-\lambda-\frac{1}{2}=k \qquad (k=0,1,...).$$

$$\sqrt{\frac{\mu a^2}{2\hbar^2\pi^2}(E+V_0)}=\frac{1}{4}\left(\sqrt{\frac{8\mu V_0 a^2}{\pi^2\hbar^2}+1}-1\right)+\frac{1+2k}{2}$$

Возводим в квадрат, сокращаем слева и справа член, обратно вводим λ, получаем:

$$E_k=\left[(2k+1)^2+4(2k+1)\lambda-2\lambda\right]\frac{\pi^2\hbar^2}{2\mu a^2}.$$

Аналогично, гипергеометрический ряд для u_2 обрывается, если

$$\nu-\lambda=l \quad (l=1,2,3,...).$$

Это также будет выполняться, если будет $2k+1=2n$, тогда (??? думаю, у авторов просто ошибка в формуле ниже. или не знаю, нет вариантов, я не понял этот переход тут(???? там в пределе осциллятор по моей логике не выходит, а логику авторов не понимаю пока))

$$E_n=\left(n^2+4n\lambda-2\lambda\right)\frac{\pi^2\hbar^2}{2\mu a^2} \quad (n=1,2,3,...).$$

$$\psi_{n\text{odd}}=c_n\left(\sin\frac{\pi x}{a}\right)^{-2\lambda}F\left(-\frac{n}{2}-2\lambda,\frac{n}{2},\frac{1}{2};\cos^2\frac{\pi x}{a}\right),$$
$$\psi_{n\text{even}}=c_n(\sin\frac{\pi x}{a}\Big)^{-2\lambda}\cos\frac{\pi x}{a}F\left(-\frac{n}{2}-2\lambda+\frac{1}{2},\frac{n}{2}+\frac{1}{2},\frac{3}{2};\cos^2\frac{\pi x}{a}\right).$$

Нормированная волновая функция основного состояния

$$\varphi=\sqrt{\frac{\pi\Gamma(2\lambda+1)}{a\Gamma\left(\frac{1}{2}\right)\Gamma\left(2\lambda+\frac{3}{2}\right)}}\left(\sin\frac{\pi x}{a}\right)^{2\lambda+1},$$

тут $\Gamma\left(\frac{1}{2}\right)=\sqrt{\pi}$. (??? видимо, как-то из свойств гипергеом функции это следует.)

В предельном случае $V_0\to 0$ задача сводится к задаче с частицей в потенциальном ящике. Имеем $\lambda\to 0$ и

$$E_n=\frac{\pi^2\hbar^2}{2\mu a^2}n^2.$$

В противоположном случае $\lambda\gg 1$ для низших уровней ($n\ll\lambda$)

$$E_n=\hbar\omega\left(n+\frac{1}{2}\right) \quad (n=1,2,...),$$

(???? у меня проблема, что получается $E_n=\hbar\omega\left(n-\frac{1}{2}\right)$, не представляю вообще, откуда там плюс???) где $\omega=\frac{\pi}{a}\sqrt{\frac{2V_0}{\mu}}$. Этот же результат можно получить, разлагая потенциальную энергию вблизи точки $x=\frac{a}{2}$ и ограничиваясь квадратичными членами, ибо в этом случае у нас просто осциллятор.

ГК-1.14. Вид уравнения

Написать уравнение Шредингера в «p» представлении для частицы, движущейся в периодическом потенциальном поле $V(x) = V_0 \cos bx$.

Solution.

Оператор Гамильтона при данном потенциале имеет вид

$$\hat{H} = \frac{1}{2\mu}p^2 + \frac{1}{2}V_0 e^{b\hbar\frac{\partial}{\partial p}} + \frac{1}{2}V_0 e^{-b\hbar\frac{\partial}{\partial p}}.$$

Так как

$$e^{b\hbar\frac{\partial}{\partial p}}a(p) = a(p + b\hbar),$$

то уравнение Шредингера будет представлено в виде уравнения в конечных разностях

$$\frac{1}{2\mu}p^2 a(p) + \frac{1}{2}V_0 a(p + b\hbar) + \frac{1}{2}V_0 a(p - b\hbar) = Ea(p).$$

(?? и что с ним делать??)

ГК-1.15. Вид уравнения

Написать уравнение Шредингера в «p» представлении для частицы, движущейся в периодическом потенциальном поле $V(x) = V(x + b)$

Solution.

Это обычное уравнение, только Фурье для потенциала для периодического поля - это ряд:

$$\frac{h^2}{2\mu}k^2 a(k) + \sum_{-\infty}^{+\infty} V_n a\left(k + \frac{2\pi n}{b}\right) = Ea(k)$$

$$\left(k = \frac{p}{b}, V(x) = \sum_{-\infty}^{+\infty} V_n e^{-\frac{2\pi n i x}{b}}, V_n = V_{-n}^*\right)$$

17.1.17 Problems about solutions by special functions 2

ГК-1.16. Потенциалы - стена башенок

Определить зоны разрешенной энергии для частицы, движущейся в периодическом потенциальном поле, изображенном на рис. ниже:

Исследовать предельный случай $V_0 \to \infty$, $b \to 0$ при условии, что $V_0 b = \text{const}$.

Solution.

(??? потом подумаю про это, это почти модель Кронинга-Пенни, итоговый график почти такой же)
Волновая функция в области ямы $0 < x < a$ имеет вид

$$\psi = c_1 e^{ix_1 x} + c_2 e^{-ix_2 x}, \quad x_1 = \frac{\sqrt{2\mu}}{\hbar}$$

а в области барьера $-b < x < 0$

$$\psi = c_3 e^{ix_\beta \mathcal{D}} + c_4 e^{-ix_3 \mathcal{D}}, \quad x_2 = \frac{\sqrt{2\mu\,(E - V_0)}}{b}$$

Так как $\psi(x) = \text{const} \cdot \psi(x + l)$ (const равна по модулю единице, $l = a + b$), то в области следующего барьера $a < x < < a + b$

$$\psi = e^{ikl}\left(c_3 e^{ix_9(x-l)} + c_4 e^{-ix_2(x-l)}\right).$$

Из требования непрерывности волновой функции и ее первой производнои в точках $x = 0, x = a$ получаем четыре уравнения:

$$c_1 + c_2 = c_3 + c_4$$
$$c_1 e^{ix_1 a} + c_2 e^{-ix_1 a} = e^{ikl}\left(c_3 e^{-ix_3 b} + c_4 e^{ix_3 b}\right)$$
$$x_1\,(c_1 - c_2) = x_2\,(c_3 - c_4)$$
$$x_1\left(c_1 e^{ix_1 a} - c_2 e^{-ix_1 a}\right) = x_2\left(c_3 e^{-ix_2 b} - c_4 e^{ix_3 b}\right) e^{ikl}$$

Эта система имеет нетривиальное решение только тогда, когда

$$\cos kl = \cos x_1 a \cdot \cos x_2 b - \frac{x_1^2 + x_2^2}{2x_1 x_2} \sin x_1 a \cdot \sin x_2 b$$

Исследуем два случая: а) $E < V_0, x_2$ - мнимая величина.
Введя обозначение $x_2 = i\gamma,$ перепишем уравнение (1) в виде

$$\cos kl = \cos x_1 a \cdot \operatorname{ch} xb + \frac{x^2 - x_1^2}{2x_1 x} \sin x_1 a \cdot \operatorname{sh} xb.$$

ГК-1.18.б) Спектр в $\operatorname{ctg}^2 \frac{\pi}{a}$

Определить в квазиклассическом приближении спектр энергии частицы в поле:
$V = V_0 \operatorname{ctg}^2 \frac{\pi}{a} x (0 < x < a)$.

Solution.

(Есть пример решенной аналогичной, см. пока его, по идее по аналогии сделать прокатит)

Ответ: $E_n = \frac{\pi^2 h^2}{2\mu a^2}\left[\sqrt{\frac{2\mu a^2 V_0}{\pi^2 h^2}} + \left(n + \frac{1}{2}\right)\right]^2 - V_0$ $(n = 0, 1, 2, ...)$.

ГК-1.19. Средняя кинетическая энергия в квазиклассике

Определить в квазиклассическом приближении среднее значение кинетической энергии стационарного состояния. Система одномерная и имеется некоторая потенциальная яма.

Solution.

(?????)
Среднее значение кинетической энергии в стационарном состоянии ψ_n (волновая функция предполагается вещественной)

$$\bar{T} = -\frac{h^2}{2\mu}\int \psi_n \frac{d^2\psi_n}{dx^2} dx = \frac{\hbar^2}{2\mu}\int \left(\frac{d\psi_n}{dx}\right)^2 dx.$$

В квазиклассическом приближении в классически доступной области $(a < x < b)$ волновая функция имеет вид

$$\psi_n = \frac{A_n}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_a^x p dx - \frac{\pi}{4}\right), \quad p = \sqrt{2\mu\,(E_n - V)},$$

откуда

$$\frac{d\psi_n}{dx} = -\frac{\sqrt{p}}{\hbar} A_n \sin\left(\frac{1}{\hbar}\int_a^x p dx - \frac{\pi}{4}\right) - \frac{1}{2}\frac{A_n}{p^{3/2}}\frac{dp}{dx}\cos\left(\frac{1}{\hbar}\int_a^x p dx - \frac{\pi}{4}\right).$$

При подстановке этого выражения в интеграл, определяющий $\bar{T}$, пределы интегрирования можно ограничить классически доступной областью, так как вне этой области ψ_n экспоненциально у бывает. Заменяя квадраты сильно осциллирующих тригонометрических функций на их среднее значение $\frac{1}{2}$ и пренебрегая слагаемым $\sin\left(\frac{1}{\hbar}\int\limits_a^x pdx - \frac{\pi}{4}\right)\cdot\cos\left(\frac{1}{\hbar}\int\limits_a^x pdx - \frac{\pi}{4}\right) = \frac{1}{2}\sin\left(\frac{2}{\hbar}\int\limits_a^x pdx - \frac{\pi}{2}\right)$, потому что оно сильно осциллирует, получаем:

$$\bar{T} = \frac{A_n^2}{4\mu}\int\limits_a^b \left[p + \frac{\hbar^2}{4p^3}\left(\frac{dp}{dx}\right)^2\right]dx$$

Условие применимости квазиклассического приближения $|\frac{d\hbar}{dx}| = \frac{\hbar}{p^2}|\frac{dp}{dx}| \ll 1$ означает, что второй член под знаком интеграла мал по сравнению с первым, поэтому получаем интеграл, который вычисляется условием квантования:

$$\bar{T} = \frac{A_n^2}{4\mu}\int\limits_a^b pdx = \frac{A_n^2}{4\mu}\pi\hbar\left(n+\frac{1}{2}\right).$$

Постоянная A_n определяется из условия нормировки:

$$\int \psi_n^2 dx \approx A_n^2\int\limits_a^b \frac{1}{p}\cos^2\left(\frac{1}{\hbar}\int\limits_a^x pdx - \frac{\pi}{4}\right)dx \approx \frac{A_n^2}{2}\int\limits_a^b \frac{dx}{p} = 1.$$

Тут интеграл вычисляется с помощью условие квантования $\int\limits_a^b pdx \equiv \int\limits_a^b \sqrt{2\mu\left(E_n - V_0\right)}dx = \pi\hbar\left(n+\frac{1}{2}\right)$, для этого дифференцируем его по n, потому что все-таки у нас тут E это гладкая функция от непрерывного n, пусть и подставляем мы дискретные его значения, получаем:

$$\mu\frac{dE_n}{dn}\int\limits_a^b \frac{dx}{\sqrt{2\mu\left(E_n - V\right)}} = \mu\frac{dE_n}{dn}\int\limits_a^b \frac{dx}{p} = \pi\hbar,$$

откуда

$$A_n^2 = \frac{2\mu}{\pi\hbar}\frac{dE_n}{dn}.$$

В итоге получаем:

$$\bar{T} = \frac{1}{2}\frac{dE_n}{dn}\left(n+\frac{1}{2}\right).$$

ГК-1.20. Средняя кинетическая энергия в квазиклассике в примерах

Зная, что средняя кинетическая энергия связанного состояния $\bar{T} = \frac{1}{2}\frac{dE_n}{dn}\left(n+\frac{1}{2}\right)$, найти в квазиклассическом приближении среднюю кинетическую энергию частицы в поле:

а) $V = \frac{\mu\omega^2 x^2}{2}$

б) $V = V_0\operatorname{ctg}^2\frac{\pi x}{a}(0 < x < a)$

Solution.

Для решения задачи нужно лишь знать спектр. Для этого можно просто вспомнить ответ или решить задачу заново, см. соответствующую задачу, где сперт ищется.

Ответ: а) $\bar{T} = \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right)$;

Ответ: б) $\bar{T} = \frac{\pi^2\hbar^2}{2\mu a^2}\left[\sqrt{\frac{2\mu a^2 V_0}{\pi^2\hbar^2}} + \left(n+\frac{1}{2}\right)\right]\left(n+\frac{1}{2}\right)$.

ГК-1.21. Произвольная степень потенциала

Определить вид энергетического спектра частицы в поле $V(x) = ax^\nu$, используя квазиклассическое приближение и применяя теорему вириала.

Solution.

Из теоремы вириала следует:

$$2\bar{T} = \nu\bar{V},$$

откуда

$$E = T + V = \frac{2+\nu}{\nu}\bar{T}.$$

Подставляя в это соотношение значение средней кинетической энергии $\bar{T} = \frac{1}{2}\frac{dE_n}{dn}\left(n+\frac{1}{2}\right)$, получаем уравнение

$$E = \frac{2+v}{2v}\frac{dE}{dn}\left(n+\frac{1}{2}\right),$$

решение которого имеет вид

$$E = \text{const}\cdot\left(n+\frac{1}{2}\right)^{\frac{2\cdot\nu}{2+\nu}}.$$

ГК-1.22. Потенциал по спектру (?)

Определить вид потенциальной энергии $V(x)$ по энергетическому спектру E_n в квазиклассическом приближении. $V(x)$ считать четной функцией $V(x) = V(-x)$, монотонно возрастающей при $x > 0$. Прийти к уравнению, из которого ее можно получить.

Solution.

В качестве исходного уравнения возьмем условие квантования Бора

$$\int\limits_{x_1}^{x_2}\sqrt{2\mu[E-V(x)]}dx = \pi\hbar\left(n+\frac{1}{2}\right),$$

определяющее спектр (по крайней мере $n(E)$), если задана потенциальная энергия $V(x)$. Поскольку по условию $V(x)$ - четная функция

$$2\int\limits_{0}^{a}\sqrt{2\mu[E-V(x)]}dx = \pi\hbar\left(n+\frac{1}{2}\right), \qquad a = x_2 \equiv -x_1, \quad E = V(a)$$

Задача, таким образом, сводится к отысканию решения интегрального уравнения

$$x(V) = \frac{\hbar}{\sqrt{2\mu}}\int\limits_{E_0}^{V}\frac{dE}{\frac{dE}{dn}\sqrt{V-E}},$$

(???? вот этот переход не понял, подумал минуты 3, оставил. тут еще под корнем порядок вычитания изменился, почему???? еще раз обратную в механике задачу почитаю) где $x(V)$ - функция, обратная $V(x)$, а $\frac{dE}{dn}$ рассматривается как функция E; E_0 - начало отсчета энергии.

famous. Стационарные волновые функции в $V(x) = -Fx$

Найти волновые функции стационарных состояний одномерного движения частицы массы в однородном поле $V(x) = -Fx$ где $F = \text{const}$.

Solution..

Это известная задача, решается функцией Айри.
В уравнении Шредингера

$$\left(\frac{\hat{p}^2}{2m} - F\hat{x}\right)\Psi = e\Psi$$

оператор $\hat{p}$ возводится в квадрат, а $\hat{x}$ - в первую степень. Поэтому оно в координатном представлении является уравнением второго порядка, а в импульсном представлении - первого, следовательно, задачу удобно решать в импульсном:

$$\left[\frac{p^2}{2m} - \mathrm{i}\hbar F\frac{d}{\mathrm{d}p}\right]\Psi_E(p) = E\Psi_E(p)$$

Поскольку в однородном поле движение всегда инфинитно, энергетический спектр непрерывен.

При заданной энергии E, используя метод разделения переменных, находим решение:

$$\Psi_E(p) = C \exp\left\{\frac{\mathrm{i}p}{\hbar F}\left(E - \frac{p^2}{6m}\right)\right\}.$$

Перейдем к координатному представлению и сделаем замену $z = p/\sqrt[3]{2m\hbar F}$:

$$\begin{aligned}
\psi(x) &\sim \int\limits_{\infty}^{+\infty} \Psi(p) \exp\left(\frac{\mathrm{i}}{\hbar} px\right) \mathrm{d}p = \\
&= \int\limits_{-\infty}^{+\infty} \exp\left\{-\mathrm{i}\left[-\frac{p}{\hbar}\left(x + \frac{E}{F}\right) + \frac{p^3}{6m\hbar F}\right]\right\} \mathrm{d}p \sim \\
&\sim \int\limits_{-\infty}^{+\infty} \exp\left\{-\mathrm{i}z\left[-\sqrt[3]{\frac{2mF}{\hbar^2}}\left(x + \frac{E}{F}\right) + \frac{z^2}{3}\right]\right\} \mathrm{d}z \\
&\sim \mathrm{Ai}\left(-\sqrt[3]{\frac{2mF}{\hbar^2}}\left(x + \frac{E}{F}\right)\right)
\end{aligned}$$

где $\mathrm{Ai}(\xi)$ - функция Эйри, в интегральном представлении $\mathrm{Ai}(\xi) = \frac{1}{\sqrt{\pi}} \int\limits_0^{\infty} \cos\left(z\xi + \frac{z^3}{3}\right) \mathrm{d}z$.

Solution 2.

В рассматриваемом случае имеется только непрерывный энергетический спектр и собственные функции невырождены.

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2} - [E + Fx]\psi = 0$$

$$\frac{p^2}{2\mu}a(p) - Ea(p) = i\hbar F\frac{d}{dp}a(p).$$

Решение этого уравнения, принадлежащее собственному значению E,

$$a_E(p) = ce^{-\frac{i}{\hbar F}\left(\frac{p^3}{6\mu} - Ep\right)}$$

(???? угадываем его что ли????) представляет собой волновую функцию в импульсном представлении. Произведем нормировку функций $a(p)$ на $\delta\left(E - E'\right)$:

$$\int a_E^*(p) a_{E'}(p) dp = \delta\left(E - E'\right),$$

$$cc^* \int e^{-\frac{ip}{\hbar F}\left(E - E'\right)} dp = cc^* 2\pi\hbar F \delta\left(E - E'\right),$$

откуда

$$c = \frac{1}{\sqrt{2\pi\hbar F}}.$$

Волновая функция в координатном представлении

$$\psi(x) = \frac{\alpha}{2\pi\sqrt{F}} \int\limits_{-\infty}^{+\infty} e^{i\frac{u^3}{3} - iuq} du = \frac{\alpha}{\pi\sqrt{F}} \int\limits_0^{\infty} \cos\left(\frac{u^3}{3} - uq\right) du,$$

$$q := \left(x + \frac{E}{F}\right)\alpha, \qquad \alpha := \left(\frac{2\mu F}{\hbar^2}\right)^{1/3}.$$

этот интеграл можно выразить через функцию Эйри $\Phi(q)$:

$$\Phi(q) = \frac{1}{\sqrt{\pi}} \int\limits_0^{\infty} \cos\left(\frac{u^3}{3} + uq\right) du, \quad \psi(x) = \frac{\alpha}{\sqrt{\pi F}}\Phi(-q).$$

"Угловой" потенциал

Исследовать движение частицы в потенциале:

$$U(x) = \begin{cases} Fx, & x \geq 0 \\ \infty, & x < 0 \end{cases}$$

Solution.

Уравнение Шредингера сводится к уравнению на спецфункцию Айри, нули ее дадут спектр.
УШ есть:

$$-\frac{\hbar^2}{2m}\psi''(x) + Fx\psi(x) = E\psi(x)$$

Обезразмерим подстановкой:

$$z(x) = \frac{x - E/F}{(\hbar^2/2mF)^{1/3}}.$$

Получим уравнение Эйри:

$$\psi''(z) - z\psi(z) = 0.$$

Его общее решение - произвольная линейная комбинация функций Эйри первого и второго рода:

$$\psi(z) = C_1\,\mathrm{Ai}(z) + C_2\,\mathrm{Bi}(z)$$

Поскольку $U(x \to \pm\infty) \to \infty$, то в задаче присутствует только дискретный спектр.

При $x > 0$, уравнение совпадает с уравнением Эйри, в связи с чем его решение даётся затухающей при $x \to \infty$ функцией:

$$\psi(x) = C \cdot \mathrm{Ai}(z(x))$$

Величина $U(0) = \infty$ дает граничное условие $\psi(0) = 0$, из которого получаем корни $z_n(0)$, по ним находим спектр:

$$E_n = -z_n \left(\hbar^2 F^2/2m\right)^{1/3}$$

Список первых нулей функции Эйри $z_n \approx \{-2.3, -4.1, -5.5, ...\}$. А большие нули получим, используя асимптотику для $z \to -\infty$:

$$\sin\left(\frac{2}{3}\left(-z_n\right)^{3/2} + \frac{\pi}{4}\right) = 0 \quad \to z_n \quad \approx -\left(\frac{3\pi}{2}(n - 1/4)\right)^{2/3}$$

К примеру по этой формуле получается $z_{10} \approx -12.8281$, что отличается от численного только в 5 ой значащей цифре. Обратим внимание, что если пренебречь $1/4$ по сравнению с n то для $n = 10$ точность ухудшается в 1000 раз.

Получим

$$E_n \approx \left(\frac{9\pi^2}{8}\frac{\hbar^2 F^2}{m}\right)^{1/3} n^{2/3}$$

ПТФ-? яма $U(x) = a/(a + |x|)$

(потом решу)

Wiki. Модифицированный потенциал Пёшль - Теллера

Найти связные состояния в

$$V(x) = -\frac{\hbar^2}{2m}a^2\frac{\lambda(\lambda - 1)}{\mathrm{ch}^2\, ax}.$$

Solution.

Решаем через гипергеометрические функции, типичная на них задача.
Стационарное уравнение Шрёдингера с модифицированным потенциалом Пёшль - Теллера имеет вид:

$$-\frac{\hbar^2}{2m}\Psi''(x) - \frac{\hbar^2}{2m}a^2\frac{\lambda(\lambda - 1)}{\mathrm{ch}^2\, ax}\Psi(x) = E\Psi(x).$$

Если ввести обозначение $k = \sqrt{2mE/\hbar^2}$, то оно примет вид:

$$\Psi''(x) + \left(k^2 + a^2\frac{\lambda(\lambda-1)}{\mathrm{ch}^2\, ax}\right)\Psi(x) = 0.$$

После замены переменных

$$y = \mathrm{ch}^2\, ax$$

получим

$$y(1-y)\Psi''(y) + \left(\frac{1}{2} - y\right)\Psi'(y) - \left(\frac{k^2}{4a^2} - \frac{\lambda(\lambda-1)}{4y}\right)\Psi(y) = 0$$

Если подставить решение в виде

$$\Psi(y) = y^{\frac{\lambda}{2}}v(y),$$

то уравнение приводится к гипергеометрическому виду

$$y(1-y)v''(y) + \left(\left(\lambda + \frac{1}{2}\right) - (\lambda-1)y\right)v'(y) - \frac{1}{4}\left(\lambda^2 + \frac{k^2}{a^2}\right)v = 0$$

Обозначая

..

(дальше не выгружаю, см вики про задачу.)

Wiki. Потенциал Пёшль - Теллера

Найти стационарные состояния в потенциале Пёшль-Теллера, который имеет вид

$$U(x) = \frac{\hbar^2}{2m}a^2\left(\frac{\varkappa(\varkappa-1)}{\sin^2 ax} + \frac{\lambda(\lambda-1)}{\cos^2 ax}\right)$$

на промежутке $0 \leqslant x \leqslant \pi/(2a)$, на границе которого он обращается в бесконечность. Параметры удовлетворяют условиям $\varkappa > 1$ и $\lambda > 1$.

Solution.

(? порешаю еще раз потом)

Стационарное уравнение Шрёдингера с потенциалом Пёшль - Теллера имеет вид:

$$-\frac{\hbar^2}{2m}\Psi''(x) + \frac{\hbar^2}{2m}a^2\left(\frac{\varkappa(\varkappa-1)}{\sin^2 ax} + \frac{\lambda(\lambda-1)}{\cos^2 ax}\right)\Psi(x) = E\Psi(x)$$

Если ввести обозначение $k = \sqrt{2mE/\hbar^2}$, то оно примет вид:

$$\Psi''(x) + \left(k^2 - a^2\frac{\varkappa(\varkappa-1)}{\sin^2 ax} - a^2\frac{\lambda(\lambda-1)}{\cos^2 ax}\right)\Psi(x) = 0$$

После замены переменных

$$y = \sin^2 ax$$

получим

$$y(1-y)\Psi''(y) + \left(\frac{1}{2} - y\right)\Psi'(y) + \frac{1}{4}\left(\frac{k^2}{a^2} - \frac{\varkappa(\varkappa-1)}{y} - \frac{\lambda(\lambda-1)}{1-y}\right)\Psi(y) = 0.$$

Так как точки 0 и 1 являются особыми, то естественно представить решение в виде:

$$\Psi(y) = y^\mu(1-y)^\nu f(y)$$

Если выбрать

$$\mu = \frac{\varkappa}{2}, \quad \nu = \frac{\lambda}{2},$$

то уравнение приведётся к гипергеометрическому виду:

$$y(1-y)f''(y) + \left(\left(\varkappa + \frac{1}{2}\right) - y(\varkappa+\lambda+1)\right)f'(y) + \frac{1}{4}\left(\frac{\varkappa^2}{a^2} + (\varkappa+\lambda)^2\right)f(y) = 0.$$

Общее решение данного уравнения может быть выражено через гипергеометрические функции:

$$f(y) = C_1\,{}_2F_1(a,b;c;y) + C_2 y^{1-c}\,{}_2F_1(a+1-c, b+1-c; 2-c; y),$$

где введены обозначения:

(дальше не выгружаю, ибо мб это не нужно. мб догружу, если понадобится)

Используется как приближение для энергии двухатомной молекулы, альтернативный потенциалу Морзе.

(в других задачах тоже укажу в конце применения их, если узнаю!)

Я. Частица в треугольнике (????)

Определить уровни энергии частицы в равностороннем треугольнике.

Solution.

(задумался про это, мб почитаю статью про это, все гуглится, просто не до этого. интересная задача!)
(?? мб это в адиабатике решаться должно, там всякая геометрия, пока не уверен, где это стоит решать???)

17.1.18 Problems about radiation

Время жизни частицы на 9м уровне в колодце (???)

Найти время жизни частицы, находящейся на девятом возбужденном уровне в бесконечно глубокой потенциальной яме ширины, $a (0 < \mathrm{x} < a)$.

Solution

(задача это бред, забил на нее и все.)
(?? можно было бы попытаться теорию спонтанного излучения применить для колодца, однако какое одномерное квантовое поле??? или в пространстве какой размерности мы находимся?)
(?? какое вообще квантовое поле при любой размерности??)

Б-2.13.1 Матричные элементы водорода

Вычислить матричные элементы $\langle 2p|\hat{\mathrm{x}}|1s\rangle, \langle 2p|\hat{\mathrm{y}}|1s\rangle$ и $\langle 2p|\hat{\mathrm{z}}|1s\rangle$ для атома водорода. Какие правила отбора они определяют?

Solution

2.13.1. $\langle 210|\hat{x}|100\rangle = 0, \langle 210|\hat{\mathrm{y}}|100\rangle = 0, \langle 210|\hat{\mathrm{z}}|100\rangle = \frac{128\sqrt{2}}{243}$, $\langle 21 \pm 1|\hat{x}|100\rangle = \pm\frac{128}{243}, \langle 21 \pm 1|\hat{y}|100\rangle = i\frac{128}{243}, \langle 21 \pm 1|\hat{\mathrm{z}}|100\rangle = 0$. (Ответы приведены в атомной системе единиц.)

Б-2.13.2 Матричные элементы водорода

Вычислить матричные элементы $\langle 2p|\hat{\mathrm{p}}_x|1s\rangle$, $\langle 2p|\hat{\mathrm{p}}_y|1s\rangle$ и $\langle 2p|\hat{\mathrm{p}}_z|1s\rangle$. Какие правила отбора они определяют?

Solution

2.13.2. $\langle 210|\hat{\mathrm{p}}_x|100\rangle = 0, \langle 210|\hat{\mathrm{p}}_y|100\rangle = 0, \langle 210|\hat{\mathrm{p}}_z|100\rangle = i\frac{16\sqrt{2}}{81}$,
$\langle 21\pm1|\hat{\mathrm{p}}_x|100\rangle = \pm i\frac{16}{81}, \langle 21\pm1|\hat{\mathrm{p}}_y|100\rangle = -\frac{16}{81}, \langle 21\pm1|\hat{\mathrm{p}}_z|100\rangle = 0$. (Ответы приведены в атомной системе единиц.)
(???? что с правилами отбора???)

Б-2.13.3 Угловое распределение излучения водорода

Найти угловое распределение фотонов, излучающихся в переходе $|2p\rangle \to |1s\rangle$ атома водорода, и время жизни $|2p\rangle$ состояния. Выразить это время в атомных единицах времени.

Solution

2.13.3. Уравнение Шредингера, описывающее атом водорода, взаимодействующий с вторично-квантованным полем фотонов, имеет вид

$$\left\{ i\hbar\frac{\partial}{\partial t} - \hat{\mathrm{H}}^{(0)} - \hat{\mathrm{V}} \right\} |\Psi\rangle = 0, \quad \hat{\mathrm{V}} = \frac{e}{mc}(\mathbf{A}\hat{\mathbf{p}}), \quad -e < 0.$$

Здесь $\hat{\mathrm{H}}^{(0)} = \hat{\mathbf{p}}^2/(2m) - e^2/r$ - гамильтониан атома водорода, $\hat{\mathrm{V}}$ - оператор возмущения. Возмущение периодически зависит от времени, потому что вектор-потенциал фотонного поля (11.70) записывается так:

$$\hat{\mathbf{A}}(\mathbf{r},t) = \sum_{\mathbf{k},\lambda} \sqrt{\frac{2\pi\hbar c^2}{\omega L^3}} \left\{ \mathbf{e}_{\mathbf{k},\lambda} \hat{\mathrm{c}}_{\mathbf{k},\lambda} e^{-i(\omega t - \mathrm{kr})} + \mathbf{e}^*_{\mathbf{k},\lambda} \hat{\mathrm{c}}^+_{\mathbf{k},\lambda} e^{i(\omega t - \mathbf{kr})} \right\}$$

где $\hat{c}^+_{\mathbf{k},\lambda}$и $\hat{c}_{\mathbf{k},\lambda}$ - операторы рождения и уничтожения фотона с волновым вектором $\mathbf{k}$ и состоянием поляризации $\lambda = 1, 2$, а $\mathbf{e}_{\mathbf{k},\lambda}$ - единичный вектор поляризации. Вектор-потенциал $\hat{\mathbf{A}}(\mathbf{r},t)$ нормирован на объем $V = L^3$, потому что поле фотонов рассматривается в кубе с длиной ребра L при циклических граничных условиях.

Рассмотрим квантовый переход, совершаемый атомом водорода из состояния $2p$ в состояние $1s$, который сопровождается излучением одного фотона с волновым вектором $\mathbf{k}$ и поляризацией λ. Фотон излучается из вакуума, поэтому мы имеем дело с процессом спонтанного излучения. Начальное и конечное состояния полной квантовой системы, включающей атом и электромагнитное поле, имеют вид $|i\rangle = |2p; 0, 0, ..., 0\rangle$ и $|f\rangle = |1s; \mathbf{1}_{\mathbf{k},\lambda}, 0, ..., 0\rangle$, причем $\mathbf{1}_{\mathbf{k},\lambda}$ - число заполнения, отвечающее наличию одного фотона.

Поскольку $\langle \mathbf{1}_{\mathbf{k},\lambda}, 0, ..., 0|\hat{c}^+_{\mathbf{k},\lambda}|0, 0, ..., 0\rangle = 1$, то в матричный элемент оператора возмущения $\langle f|\hat{V}|i\rangle$, отвечающий нашему процессу, вносит вклад только одно слагаемое из суммы (2), которое включает оператор рождения $\hat{c}^+_{\mathbf{k},\lambda}$и зависит от времени, как $e^{i\omega t}$. Поэтому дифференциальная вероятность нашего квантового перехода в единицу времени запишется следующим образом (см. (II.50)):

$$dw^{\lambda}_{if} = \frac{2\pi}{\hbar} |\langle f|\hat{\mathrm{V}}^+_{\mathbf{k},\lambda}|i\rangle|^2 \delta\left(E_f - E_i + \hbar\omega\right) d\nu_f,$$

$$\hat{\mathrm{V}}^+_{\mathbf{k},\lambda} = \frac{e}{m}\sqrt{\frac{2\pi\hbar}{\omega L^3}} e^{-i\mathbf{kr}} \left(\mathbf{e}^*_{\mathbf{k},\lambda}\hat{\mathbf{p}}\right),$$

где E_i и E_f - начальная и конечная энергия атома водорода (для состояний $2p$ и $1s$). В этой формуле предполагается далее провести интегрирование по энергии конечных фотонов.

Учитываем, что

$$d\nu_f = \frac{d^3k}{(2\pi)^3} L^3 = \frac{k^2 dk d\Omega}{(2\pi)^3} L^3 = \frac{\omega^2 d(\hbar\omega)}{\hbar c^3 (2\pi)^3} L^3 d\Omega,$$

так как энергия фотона $E_{\mathbf{k}} = \hbar\omega = \hbar kc$, и $dk = d\omega/$. Интегрируя в (3)

$$dW^{\lambda}_{ij} = \frac{e^2}{\hbar c}\frac{\omega_{if}}{2\pi} |\frac{\left(\mathbf{e}^*_{\mathbf{k},\lambda}\mathbf{p}_{ii}\right)}{mc}|^2 d\Omega, \quad \text{где} \quad \mathbf{p}_{fi} = \langle 2p|e^{-i\mathbf{kr}}\hat{\mathbf{p}}|1s\rangle$$

и мы ввели обозначение $\omega_{if} = \left(E_i - E_f\right)/\hbar$. Поскольку характерное значение величины $(\mathbf{kr}) \sim ka \sim \hbar\omega a/(\hbar c) \sim e^2/a \cdot a/(\hbar c) \sim \alpha \simeq 1/137 \ll 1$, т. е. является малым для атомных процессов, то можно разложить экспоненту в (4) и пренебречь величиной $(\mathbf{kr})$ по сравнению с единицей [9]. Учитывая, кроме того, что

$$\frac{1}{m}\mathbf{p}_{fi} = -i\omega_{if}\mathbf{r}_{fi},$$

видим, что матричный элемент оператора возмущения сводится к матричному элементу оператора дипольного электрического момента $\hat{\mathbf{d}} = -\hat{\mathbf{r}}$. В итоге мы получаем дифференциальную вероятность перехода в дипольном приближении

$$dW^{\lambda}_{if} = \frac{\omega^3_{ij}}{2\pi\hbar c^3} |\left(\mathbf{e}^*_{\mathbf{k},\lambda}\mathbf{d}_{ii}\right)|^2 d\Omega.$$

В формуле (5) необходимо провести суммирование по поляризациям конечных фотонов при помощи формулы

$$\sum_{\lambda=1,2} \left(\mathbf{e}_{\mathrm{k},\lambda}\right)_i \left(\mathbf{e}^*_{\mathbf{k},\lambda}\right)_j = \delta_{ij} - \frac{k_i k_j}{k^2}$$

В результате получим угловое распределение вероятности излучения:

$$dW_{if} = \frac{\omega^3_{if}}{2\pi\hbar c^3} ||\mathbf{k}^0 \times \mathbf{d}_{it}||^2 d\Omega,$$

где $\mathbf{k}^0 = \mathbf{k}/|\mathbf{k}|$. Интегрируя в (7) по угловым переменным [10], получаем полную вероятность излучения фотонов, сопровождающего переход атома $2p \to 1s$:

$$W_{if} = \frac{4}{3}\frac{\omega^3_{if}}{\hbar c^3} |\mathbf{d}_{fi}|^2.$$

Воспользуемся далее результатами задачи 2.13.1 и увидим, что

$$|\mathbf{d}_{ii}|^2 = e^2|\langle 2p|\hat{\mathbf{r}}|1s\rangle|^2 = e^2\left[|\langle 2p|\hat{x}|1s\rangle|^2 + |\langle 2p|\hat{y}|1s\rangle|^2 + |\langle 2p|\hat{z}|1s\rangle|^2\right] = \left(\frac{128\sqrt{2}}{243}ea\right)^2,$$

независимо от значения квантового числа $m = 0, \pm 1$ начального состояния $\left(a = \hbar^2/(\text{ те } e^2\right)$ - боровский радиус). Имея также в виду, что $\hbar\omega_{if} = E_2 - E_1 = 3e^2/(8a)$, находим из формулы (8)

$$W_{if} = \left(\frac{2}{3}\right)^8 \alpha^4 \frac{c}{a}, \quad \text{где } \alpha = \frac{e^2}{\hbar c} \simeq \frac{1}{137}$$

- постоянная тонкой структуры. Подставляя численные значения физических величин, получаем, что вероятность $W_{if} \simeq 6,35 \cdot 10^8 \text{с}^{-1}$, время жизни $2p$-состояния $\tau \simeq 1,57 \cdot 10^{-9}$ с или $\tau = (3/2)^8 \alpha^{-3} \tau_{\text{ат}}$, где $\tau_{\text{ат}} = \hbar a/e^2 = 2,4 \cdot 10^{-17}$с - атомная единица времени.

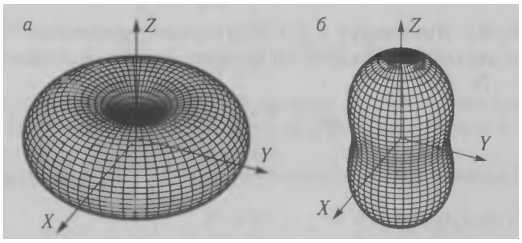
Наконец, проведем анализ углового распределения излученных фотонов. Оно будет различным для начальных состояний атома водорода с квантовыми числами $m = 0$ и $m = \pm 1$ (рисунки 2.17, а и б). Обозначим через φ и θ сферические углы волнового вектора $\mathbf{k}$. Учитывая значения матричных элементов оператора $\hat{\mathbf{d}}$ для начальных состояний $m = 0$ и $m = \pm 1$ (задача 2.13.1), получаем на основе формулы (7)

$$dW_{if}|_{m=0} = W \sin^2\theta d\Omega, \quad dW_{if}|_{m=\pm 1} = W \cdot \frac{1}{2}\left(1 + \cos^2\theta\right) d\Omega,$$

где при помощи W мы обозначили величину

$$W' = \frac{\omega_{if}^3}{2\pi\hbar c^3}|\mathbf{d}_{it}|^2 = \frac{3}{8\pi}W_{if}.$$

Заметим, что для вывода соотношений (9) можно использовать формулу $|\left[\mathbf{k}^0 \times \mathbf{d}_{ii}\right]|^2 = (\mathbf{d}_{ii}^* \mathbf{d}_{ji}) - \left(\mathbf{k}^0 \mathbf{d}_{ji}^*\right)\left(\mathbf{k}^0 \mathbf{d}_{ji}\right)$. Интегрирование по углам в выражениях (9) в обоих случаях дает один и тот же результат (8).



(??? пока это ещё не понимаю.)

Б-2.13.4 Время параллельности спина полю

Нейтрон находится в однородном магнитном поле $\mathcal{H}_0 \| z$. Определить время жизни состояния с проекцией спина на направление поля $m_s = +1/2$. Получить численное значение времени жизни для $\mathcal{H}_0 = 1$ кГс.

Solution

Нейтрон - электрически нейтральная частица со спином 1/2, обладающая собственным магнитным моментом $\mu = -\mu_n = -1,913\mu_8$, где $\mu_{\text{R}} = e\hbar/(2m_p c)$ - ядерный магнетон.

Взаимодействие нейтрона с электромагнитным полем (с классическим внешним и вторично-квантованным полем излучения) имеет вид

$$\hat{\text{V}} = -\hat{\mu}\left(\mathcal{H}_0 + \hat{\mathcal{H}}_{rad}\right),$$

где $\hat{\mu} = -\mu_n \hat{\sigma}$,

$$\hat{\mathcal{H}}_{\text{rad}} = \text{rot}\,\hat{\mathbf{A}}_{\text{rad}} = i\sum_{\mathbf{k},\lambda}\sqrt{\frac{2\pi\hbar c^2}{\omega L^3}}\left\{\left[\mathbf{k} \times \mathbf{e}_{\mathbf{k},\lambda}\right]\hat{c}_{\mathbf{k},\lambda}e^{-i(\omega t - \mathbf{kr})} - \left[\mathbf{k} \times \mathbf{e}_{\mathbf{k},\lambda}^*\right]\hat{c}_{\mathbf{k},\lambda}^+ e^{i(\omega t - \mathbf{kr})}\right\},$$

где мы воспользовались формулой (II.70). Гамильтониан невозмущенной задачи записывается в виде: $\hat{\mathrm{H}}^{(0)} = -\hat{\mu}\mathcal{H}_0 = \mu_n\hat{\sigma}\mathcal{H}_0 = \mu_n\hat{\sigma}_z\mathcal{H}_0$, так как ось z направлена вдоль поля $\mathcal{H}_0$. Волновые функции, собственные для невозмущенного гамильтониана:

$$\chi_1 = \chi_{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_2 = \chi_{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Эти функции отвечают уровням энергии невозмущенного гамильтониана $E^{(0)}_{1,2} = \pm\mu_n\mathcal{H}_0$. Как видно, энергия нейтрона в магнитном поле зависит от ориентации магнитного момента по отношению к направлению поля. Причем два разных состояния ориентации магнитного момента обладают различной устойчивостью в отношении взаимодействия с полем фотонов. Поэтому оказываются возможными спонтанные переходы нейтрона между состояниями, отличающимися ориентацией магнитного момента. Такие переходы сопровождаются изменением ориентации спина и одновременным испусканием фотона. Это и есть излучение магнитного момента нейтрона во внешнем магнитном поле.

В нашем случае возможен переход нейтрона из состояния $\gamma 1$ в состояние χ_2, которое обладает бóльшей устойчивостью. Проводя начальные преобразования по аналогии с задачей 2.13.3, мы можем записать дифференциальную вероятность излучения фотона с волновым вектором k и поляризацией λ в виде

$$dW^{\lambda}_{12} = \frac{2\pi}{\hbar}|V_{21}|^2 d\nu_f = \frac{\omega_{12}}{2\pi\hbar c}|\left[\mathbf{k}\times\mathbf{e}^*_{\mathbf{k},\lambda}\right]\mu_{21}|^2 d\Omega,$$

где мы ввели обозначения $\omega_{12} = 2\mu_n\mathcal{H}_0, \mu_{21} = \mu_n\langle\chi_2|\hat{\sigma}|\chi_1\rangle$. Выражение dW^{λ}_{12} можно переписать в виде

$$dW^{\lambda}_{12} = \frac{\omega_{12}}{2\pi\hbar c}|\mathbf{e}^*_{\mathbf{k},\lambda}\mathbf{m}_{21}|^2 d\Omega, \quad \text{где} \quad \mathbf{m}_{21} = [\mathbf{k}\times\boldsymbol{\mu}_{21}].$$

Далее суммируем по поляризациям излученных фотонов, как в задаче 2.13.3. В итоге получаем

$$dW_{12} = \frac{\omega^3_{12}}{2\pi\hbar c^3}|\left[\mathbf{k}^0\times\boldsymbol{\mu}_{21}\right]|^2 d\Omega,$$

где $\mathbf{k}^0 = \mathbf{k}/k$, и мы учли, что $\mathbf{k}|\mathbf{k}\times\boldsymbol{\mu}_{21}] = 0$. Интегрируем по углам вылета фотона так же, как и в задаче 2.13.3, и находим полную вероятность излучения в единицу времени:

$$W = \frac{4}{3}\frac{\omega^3_{12}}{\hbar c^3}|\boldsymbol{\mu}_{21}|^2.$$

Очевидно, что излучение имеет магнитно-дипольный характер (ср. (2) и формулу (8) задачи 2.13.3). Вычисляем матричные элементы:

$$(\mu_{21})_x = \mu_n, \quad (\mu_{2\mathrm{I}})_y = i\mu_n, \quad (\mu_{21})_z = 0$$

и получаем окончательное выражение для полной вероятности излучения, сопровождаемого переворотом спина в магнитном поле (так называемый спиновый свет нейтрона):

$$W = \frac{64}{3}\frac{\mu^5_n\mathcal{H}^3_0}{\hbar^4 c^3}.$$

Проведем численные оценки. Для напряженности поля $\mathcal{H}_0 = 1$ кГс получаем время жизни $\tau \simeq 1,9\cdot 10^{28}$с $\simeq 5,9\cdot 10^{20}$ лет. Таким образом, в лабораторных условиях вероятность данного процесса чрезвычайно мала. Однако в сверхсильных полях $\sim 10^{13}$Гс, существующих вблизи астрофизических объектов таких, как нейтронные звезды, вероятность может сильно возрасти, при этом время время жизни τ может составить ~ 10 с.

Б-2.13.5 Фотоэффект в рамках квантовой механики (!??!?!?)

Найти сечение фотоэффекта на атоме водорода под действием плоской монохроматической волны с частотой ω для случая $\hbar\omega \gg I$, где I - потенциал ионизации атома. Сравнить результаты вычислений при классическом и квантовом описаниях падающей электромагнитной волны.

Solution.

Пишем правило Ферми, подставляем начальное и конечное состояния. (??? так просто???)

Фотоэффектом называется реакция “выбивания” электрона из атома падающим фотоном (в задаче речь идет о фотоэффекте на атоме водорода).

В соответствии с условием задачи полагаем, что в начальном состоянии в системе находятся один фотон и атом водорода в основном состоянии, т. е. $|i\rangle = |Is; \mathbf{1}_{\mathbf{k},\lambda}, 0, 0, ..., 0\rangle$, а конкретно

$$E_l = E_1 = -\frac{e^2}{2a}, \quad \psi_i = \psi_{100}(r) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

- энергия и волновая функция основного состояния атома водорода, $a = \hbar^2/\left(me^2\right)$ - радиус боровской орбиты. Атом взаимодействует с вторично-квантованным полем фотонов, описываемым вектор-потенциалом $\hat{\mathbf{A}}(\mathbf{r}, t)$ (см. (II.70)). Оператор, описывающий взаимодействие, имеет обычный вид:

$$\hat{\mathrm{V}} = \frac{e}{mc}(\hat{\mathbf{A}}\hat{\mathbf{p}})$$

и играет роль оператора возмущения в рассматриваемой задаче ($-e < 0$ - заряд электрона). В результате акта взаимодействия происходит ионизация атома, т. е. атомный электрон переходит в непрерывный спектр. Энергия ионизации в данном случае равна $I = -E_1 = e^2/(2a)$.

Далее мы предположим, что энергия вылетающего из атома электрона велика по сравнению с I, а это значит, что электрон является быстрым, следовательно, можно пренебречь влиянием атома на состояние электрона и выбрать конечное состояние системы в виде $|f\rangle = |\mathbf{p}; 0, 0, ..., 0\rangle$, а конкретно

$$E_f = \frac{\mathbf{p}^2}{2m}, \quad \psi_f = \psi_{\mathbf{p}}(\mathbf{r}) = \frac{1}{\sqrt{L^3}} e^{\frac{i}{\hbar}\mathbf{p}}$$

- энергия и волновая функция свободного электрона. Вероятность процесса в единицу времени, во время которого система поглощает энергию радиационного поля, рассчитывается согласно формуле (см. (II.50))

$$dw_{if} = \frac{2\pi}{\hbar}|V_{fi}|^2 \delta\left(E_i - E_f + \hbar\omega\right) d\nu_f,$$

где E_i и E_l - начальная и конечная энергии электрона, а в матричный элемент $V_{fi} = \langle f|\hat{V}|i\rangle$ вносит вклад только одно слагаемое из суммы (II.70), включающее оператор уничтожения $\hat{c}_{\mathbf{k},\lambda}$, так что $\langle 0, 0, ..., 0|\hat{c}_{\mathbf{k},\lambda}|\mathbf{1}_{\mathbf{k},\lambda}, 0, ..., 0\rangle = 1$. Поэтому $V_{fi} = \langle f|\hat{V}_{\mathbf{k},\lambda}|i\rangle$, где

$$\hat{\mathrm{V}}_{\mathbf{k},\lambda} = \frac{e}{m}\sqrt{\frac{2\pi\hbar}{\omega L^3}} e^{i\mathbf{kr}} \left(\mathbf{e}_{\mathbf{k},\lambda}\hat{\mathbf{p}}\right).$$

Поскольку для волновой функции (1) мы использовали нормировку на объем куба периодичности L^3, то связь дифференциальной вероятности перехода с дифференциальным сечением определяется соотношением

$$d\sigma = \frac{dW}{j} = L^3 \frac{dW}{v} = L^3 \frac{dW}{c},$$

где $\mathbf{j} = \mathbf{v}/L^3$ - плотность потока вероятности при нашем выборе нормировки (для падающих фотонов, очевидно, $v = c$). Запишем матричный элемент:

$$V_{fi} = \frac{e}{mL^3}\sqrt{\frac{2\hbar}{\omega a^3}}\mathbf{e}_{\mathbf{k},\lambda} \int e^{-\frac{i}{\hbar}\mathbf{pr} + i\mathbf{krp}} \hat{\mathbf{p}} e^{-r/a} d^3x.$$

В этом выражении можно пренебречь импульсом фотона по сравнению с импульсом электрона, имея в виду, что из закона сохранения энергии (см. (2)) следует

$$\hbar\omega = I + \frac{\mathrm{p}^2}{2m} \simeq \frac{\mathrm{p}^2}{2m} \ll mc^2,$$

т. е. мы считаем электрон нерелятивистским, а поэтому

$$\frac{\hbar k}{p} \sim \left(\frac{\hbar\omega}{2mc^2}\right)^{1/2} \ll 1.$$

При вычислении интеграла в (5) удобно вначале проинтегрировать по частям, имея в виду, что $\hat{\mathrm{p}} = -i\hbar\nabla$ и перенести действие производной на плоскую волну. Кроме того необходимо учесть, что $\hbar\omega \gg I$, откуда следует, что $pa/\hbar \gg 1$. Расчет интеграла при этом условии дает

$$\frac{8\pi\hbar^4}{ap^4}\mathbf{p}.$$

Для дальнейших вычислений заметим, что

$$d\nu_f = \frac{d^3p}{(2\pi\hbar)^3}L^3 = \frac{L^3p^2dpd\Omega}{(2\pi\hbar)^3} = \frac{L^3pd\left(p^2\right)d\Omega}{2(2\pi\hbar)^3}.$$

Подставляем теперь значение матричного элемента (5) в (2) и, учитывая (4) и (6), интегрируем по энергии конечных электронов при помощи δ-функции (берем интеграл по $d\left(p^2\right)$). В итоге дифференциальное сечение нашего процесса приобретает вид

$$d\sigma = 64\left(\frac{e^2}{\hbar c}\right)\left(\frac{\hbar^2}{me^2}\right)^2\left(\frac{I}{\hbar\omega}\right)^{7/2}|\mathbf{e}_{\mathbf{k},\lambda}\mathbf{n}|^2d\Omega,$$

где $\mathbf{n} = \mathbf{p}/p$ - единичный вектор в направлении вылета электрона. Проводим усреднение по поляризациям начального фотона в выражении (7), используя формулу (6) задачи 2.13.3, разделив результат на два. В результате получаем дифференциальное сечение фотоэффекта для неполяризованных фотонов:

$$d\sigma = 32\alpha a^2\left(\frac{I}{h\omega}\right)^{7/2}|\left[\mathbf{k}^0\times\mathbf{n}\right]|^2d\Omega,$$

где $\alpha = e^2/(\hbar c), \mathbf{k}^0 = \mathbf{k}/k$ - направление волнового вектора падающего фотона. Интегрируя по угловым переменным, получаем окончательный результат - полное сечение фотоэффекта:

$$\sigma = \frac{256}{3}\alpha a^2\left(\frac{l}{\hbar\omega}\right)^{7/2}.$$

В заключение сделаем несколько замечаний относительно полуклассического описания фотоэффекта. При таком подходе электромагнитное поле описывается классически, т. е.

$$\mathbf{A}(\mathbf{r},t) = \mathbf{A}_0e^{-i(\omega t-\mathbf{kr})} + \mathbf{A}_0^*e^{i(\omega t-\mathbf{kr})},$$

а частицы описываются методами квантовой механики. Все, сказанное о выборе начальных и конечных состояний для электрона и о приближениях остается в силе, да и (по большей части) методы решения сохраняются. В основе также лежит формула для вероятности переходов в единицу времени (2). Оператор электромагнитного взаимодействия, очевидно, имеет вид

$$\hat{\mathrm{V}} = -\frac{ie}{mc}(\mathbf{A}\hat{\nabla}).$$

Для определенности будем считать, что плоская волна распространяется вдоль оси z, а вектор электрического поля (т. е. поляризация) направлен вдоль оси x, тогда ось z совпадает с направлением вектора k, а $\mathbf{A}_0 = \{A_0, 0, 0\}$ (A_0 считаем вещественной величиной). Тогда дифференциальная вероятность переходов в единицу времени, проинтегрированная по энергиям конечных электронов, имеет вид

$$dW_{if} = \frac{mpL^3}{4\pi^2\hbar^4}|V_{fi}|^2d\Omega,$$
$$V_{fi} = -\frac{ie\hbar A_0}{mc}\int\frac{1}{L^{3/2}}e^{-\frac{i}{\hbar}\mathrm{pr}}\frac{\partial}{\partial x}\left[\frac{1}{\sqrt{\pi a^3}}e^{-r/a}\right]d^3x.$$

Для вычисления интеграла в (10) тоже нужно вначале проинтегрировать по частям. Сечение процесса равно дифференциальной вероятности, деленной на плотность потока падающих фотонов. Усредненный по времени вектор Пойнтинга направлен вдоль оси z и равен

$$\bar{S} = \frac{c}{4\pi}\overline{|\mathcal{E}\times\mathcal{H}||} = \frac{\omega^2}{2\pi c}A_0^2,$$

а плотность потока фотонов, т. е. число фотонов, падающих в 1 секунду на единичную площадку есть $j = \bar{S}/(\hbar\omega)$. В итоге

$$d\sigma = 32\frac{e^2}{\omega mca^5}\left(\frac{\hbar}{p}\right)^7\left(\frac{p_x}{\hbar}\right)^2, \text{ где } p_x = p\cos\varphi\sin\theta.$$

Интегрирование по углам дает результат, полностью совпадающий с формулой (8).

17.2 Analysis of Typical Models

17.2.1 Problems about Spin, Two-Level Systems, and Their Measurements

ПТФ-1.з1.* Осцилляция Раби (50 б).

На двухуровневую систему накладывается периодическое поле, которое может вызывать переходы между этой парой уровней:

$$\hat{H}(t) = \begin{pmatrix} \varepsilon_1 & Ve^{-i\omega t} \\ Ve^{i\omega t} & \varepsilon_2 \end{pmatrix}$$

В начальный момент времени система находилась в состоянии $|\psi(t=0)\rangle = |\uparrow\rangle$. Определите вероятность обнаружить её в состоянии $|\downarrow\rangle$ через произвольное время t. Что происходит при резонансе, когда отстройка частоты $\delta \equiv \varepsilon_1 - \varepsilon_2 - \hbar\omega$ обращается в нуль?

Указание: покажите, что от зависимости гамильтониана от времени можно избавиться "переходом во вращающуюся систему отсчёта" (rotating wave approximation) – унитарным преобразованием (см. упражнения 2, 3) вида $\hat{U}(t) = e^{i\hat{\sigma}_z\omega_0 t}$. Чему равна соответствующая частота ω_0?

Solution.

(???)
We known that

$$U(t) = e^{i\hat{\sigma}_z\omega_0 t} = \cos\omega_0 t + i\sin\omega_0 t \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} e^{i\omega_0 t} & 0 \\ 0 & e^{-i\omega_0 t} \end{pmatrix}, \qquad U^\dagger(t) = \begin{pmatrix} e^{-i\omega_0 t} & 0 \\ 0 & e^{i\omega_0 t} \end{pmatrix};$$

$$\hat{H}' = \hat{U}\hat{H}\hat{U}^\dagger - i\hbar\hat{U}\partial_t\hat{U}^\dagger$$

thus
(??? what are we doing??)

$$\hat{H}' = \begin{pmatrix} \varepsilon_1 & Ve^{i(2\omega_0-\omega)t} \\ Ve^{-i(2\omega_0-\omega)t} & \varepsilon_2 \end{pmatrix} - \begin{pmatrix} \hbar\omega_0 & 0 \\ 0 & -\hbar\omega_0 \end{pmatrix} = \begin{pmatrix} \varepsilon_1 - \hbar\omega_0 & Ve^{i(2\omega_0-\omega)t} \\ Ve^{-i(2\omega_0-\omega)t} & \varepsilon_2 + \hbar\omega_0 \end{pmatrix}$$

Избавимся от зависимости от времени, подобрав соответствующее ω_0:

$$\omega_0 = \frac{\omega}{2}$$

$$\hat{H}' = \begin{pmatrix} \varepsilon_1 - \frac{\hbar\omega}{2} & V \\ V & \varepsilon_2 + \frac{\hbar\omega}{2} \end{pmatrix}$$

При этом переходе собственные векторы гамильтониана меняются на фазу:

$$\begin{pmatrix} |1'\rangle \\ |2'\rangle \end{pmatrix} = \begin{pmatrix} e^{i\omega_0 t} & 0 \\ 0 & e^{-i\omega_0 t} \end{pmatrix} \begin{pmatrix} |1\rangle \\ |2\rangle \end{pmatrix} = \begin{pmatrix} e^{i\omega_0 t}|1\rangle \\ e^{-i\omega_0 t}|2\rangle \end{pmatrix}$$

Собственные числа дают спектр возможных значений энергии:

$$\left(\varepsilon_1 - \frac{\hbar\omega}{2} - E\right)\left(\varepsilon_2 + \frac{\hbar\omega}{2} - E\right) - V^2 = 0$$

$$E_{1,2} = \frac{\varepsilon_1 + \varepsilon_2 \pm \sqrt{(\varepsilon_2 - \varepsilon_1 + \hbar\omega)^2 + 4V^2}}{2}$$

Соответствующие нормированные собственные состояния системы:

$$|1'\rangle = \frac{1}{C_1}\begin{pmatrix} \frac{\varepsilon_1 - \varepsilon_2 - \hbar\omega + \sqrt{(\varepsilon_2 - \varepsilon_1 + \hbar\omega)^2 + 4V^2}}{2V} \\ 1 \end{pmatrix}, \quad |2'\rangle = \frac{1}{C_2}\begin{pmatrix} \frac{\varepsilon_1 - \varepsilon_2 - \hbar\omega - \sqrt{(\varepsilon_2 - \varepsilon_1 + \hbar\omega)^2 + 4V^2}}{2V} \\ 1 \end{pmatrix}$$

$$|1\rangle = e^{-i\omega_0 t}|1'\rangle = \frac{e^{-i\omega_0 t}}{C_1}\begin{pmatrix} \frac{\varepsilon_1 - \varepsilon_2 - \hbar\omega + \sqrt{(\varepsilon_2 - \varepsilon_1 + \hbar\omega)^2 + 4V^2}}{2V} \\ 1 \end{pmatrix} = \frac{e^{-i\omega_0 t}}{C_1}\begin{pmatrix} a \\ 1 \end{pmatrix} = e^{-i\omega_0 t}\frac{a|\uparrow\rangle + |\downarrow\rangle}{C_1}$$

$$|2\rangle = e^{i\omega_0 t}|2'\rangle = \frac{e^{i\omega_0 t}}{C_2}\begin{pmatrix}\frac{\varepsilon_1-\varepsilon_2-\hbar\omega-\sqrt{(\varepsilon_2-\varepsilon_1+\hbar\omega)^2+4V^2}}{2V}\\1\end{pmatrix} = \frac{e^{i\omega_0 t}}{C_2}\begin{pmatrix}b\\1\end{pmatrix} = e^{i\omega_0 t}\frac{b|\uparrow\rangle+|\downarrow\rangle}{C_2}$$

Разложим начальное условие по стационарным состояниям:

$$|\psi(0)\rangle = |\uparrow\rangle = \frac{C_1 e^{i\omega_0 t}|1\rangle - C_2 e^{-i\omega_0 t}|2\rangle}{a-b}$$

Дальнейшая эволюция:

$$|\psi(t)\rangle = \frac{C_1 e^{i\omega_0 t}e^{-\frac{iE_1 t}{\hbar}}|1\rangle - C_2 e^{-i\omega_0 t}e^{-\frac{iE_2 t}{\hbar}}|2'\rangle}{a-b} = \frac{e^{-\frac{iE_1 t}{\hbar}}(a|\uparrow\rangle+|\downarrow\rangle) - e^{-\frac{iE_2 t}{\hbar}}(b|\uparrow\rangle+|\downarrow\rangle)}{a-b}$$

$$|\psi(t)\rangle = \frac{e^{-\frac{i(\varepsilon_1+\varepsilon_2)t}{2\hbar}}}{a-b}\left(e^{-\frac{i\sqrt{(\varepsilon_2-\varepsilon_1+\hbar\omega)^2+4V^2}t}{2\hbar}}(a|\uparrow\rangle+|\downarrow\rangle) - e^{\frac{i\sqrt{(\varepsilon_2-\varepsilon_1+\hbar\omega)^2+4V^2}t}{2\hbar}}(b|\uparrow\rangle+|\downarrow\rangle)\right)$$

$$\psi_\downarrow(t) = \langle\downarrow|\psi(t)\rangle = \frac{e^{-\frac{i(\varepsilon_1+\varepsilon_2)t}{2\hbar}}}{a-b}\left(e^{-\frac{i\sqrt{(\varepsilon_2-\varepsilon_1+\hbar\omega)^2+4V^2}t}{2\hbar}} - e^{\frac{i\sqrt{(\varepsilon_2-\varepsilon_1+\hbar\omega)^2+4V^2}t}{2\hbar}}\right)$$

Вероятность обнаружить систему в состоянии $|\downarrow\rangle$ через время t:

$$P_\downarrow(t) = |\psi_\downarrow(t)|^2 = \frac{4\sin^2\left(\frac{\sqrt{(\varepsilon_2-\varepsilon_1+\hbar\omega)^2+4V^2}t}{2\hbar}\right)}{(a-b)^2}$$

$$P_\downarrow(t) = \frac{4V^2\sin^2\left(\frac{\sqrt{(\varepsilon_2-\varepsilon_1+\hbar\omega)^2+4V^2}t}{2\hbar}\right)}{(\varepsilon_2-\varepsilon_1+\hbar\omega)^2+4V^2}$$

Случай резонанса:

$$\delta \equiv \varepsilon_1 - \varepsilon_2 - \hbar\omega = 0$$

$$P_\downarrow(t) = \sin^2\frac{Vt}{\hbar}$$

ПТФ-1.з2. Два спина (30 б).

Найдите уровни энергии и собственные состояния для следующего гамильтониана, описывающего систему двух взаимодействующих спинов $1/2$:

$$\hat{H} = -J(\vec{\sigma}_1 \otimes \vec{\sigma}_2) = -J(\hat{\sigma}_1^x \otimes \hat{\sigma}_2^x + \hat{\sigma}_1^y \otimes \hat{\sigma}_2^y + \hat{\sigma}_1^z \otimes \hat{\sigma}_2^z)$$

Solution.

$$\hat{H} = -J\left(\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix} + \begin{pmatrix}0&0&0&-1\\0&0&1&0\\0&1&0&0\\-1&0&0&0\end{pmatrix} + \begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&1\end{pmatrix}\right) = J\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix}$$

Собственные числа дают спектр возможных значений энергии:

$$E_1 = 3J, \quad E_{2,3,4} = -J$$

Соответствующие нормированные собственные состояния системы:

$$|1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\-1\\1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle), \quad |2\rangle = \begin{pmatrix}0\\0\\0\\1\end{pmatrix} = |\downarrow\downarrow\rangle$$

$$|3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle), \quad |4\rangle = \begin{pmatrix}1\\0\\0\\0\end{pmatrix} = |\uparrow\uparrow\rangle$$

Solution.

$\hat{\boldsymbol{S}} = (\hbar/2)\hat{\boldsymbol{\sigma}}$
Рассмотрим состояние $|\xi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$, матрица плотности такого состояния имеет вид:

$$\hat{\rho} = |\psi\rangle\langle\psi| = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \frac{1}{2}\left(\hat{\mathbb{I}} + \hat{\sigma}_x\right)$$

$$\langle\hat{\boldsymbol{S}}_x\rangle = (\hbar/4)\,\mathrm{Tr}\,(\hat{\rho}\hat{\sigma}_x) = \frac{1}{2}\,\mathrm{Tr}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \hbar/2,$$

$$\langle\hat{\boldsymbol{S}}_y\rangle = (\hbar/2)\frac{i}{2}\,\mathrm{Tr}\begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} = 0,$$

$$\langle\hat{\boldsymbol{S}}_z\rangle = (\hbar/2)\frac{1}{2}\,\mathrm{Tr}\begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} = 0.$$

Теперь найдем дисперсию $\langle(\boldsymbol{S} - \langle\boldsymbol{S}\rangle)^2\rangle$, (только я так и не понял, как этой формулой пользоваться, ведь для $S_x : 2\times 2$, а $\langle S_x\rangle : 1\times 1$, поэтому) воспользуемся $\sigma_S^2 = \langle S^2\rangle - \langle S\rangle^2$

$$\langle\hat{\boldsymbol{S}}_x^2\rangle = (\hbar/2)^2\frac{1}{2}\,\mathrm{Tr}\left(\hat{\rho}\,\hat{\mathbb{I}}\right) = \frac{1}{2}\,\mathrm{Tr}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = (\hbar/2)^2 \equiv \langle\hat{\boldsymbol{S}}_y^2\rangle = \langle\hat{\boldsymbol{S}}_z^2\rangle,$$

$$\sigma_x = \sqrt{(\hbar/2)^2 - (\hbar/2)^2)} = 0; \quad \sigma_y = \sigma_z = (\hbar/2); \quad \sigma_{S_1} = \sqrt{\sigma_x^2 + \sigma_y^2 + \sigma_z^2} = \sqrt{2}(\hbar/2).$$

Теперь рассмотрим состояние $\hat{\rho}_2 = \left(\hat{\mathbb{P}}_\uparrow + \hat{\mathbb{P}}_\downarrow\right)/2$, для которого

$$\hat{\rho}_2 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}\hat{\mathbb{I}}$$

$$\langle\hat{\boldsymbol{S}}_x\rangle = (\hbar/4)\,\mathrm{Tr}\,(\hat{\rho}_2\hat{\sigma}_x) = \frac{1}{2}\,\mathrm{Tr}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = 0,$$

$$\langle\hat{\boldsymbol{S}}_y\rangle = (\hbar/2)\frac{i}{2}\,\mathrm{Tr}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = 0,$$

$$\langle\hat{\boldsymbol{S}}_z\rangle = (\hbar/2)\frac{1}{2}\,\mathrm{Tr}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = 0.$$

Дисперсию считаем как:

$$\langle\hat{\boldsymbol{S}}_x^2\rangle = (\hbar/2)^2\frac{1}{2}\,\mathrm{Tr}\left(\hat{\rho}\,\hat{\mathbb{I}}\right) = \frac{1}{2}\,\mathrm{Tr}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = (\hbar/2)^2 \equiv \langle\hat{\boldsymbol{S}}_y^2\rangle = \langle\hat{\boldsymbol{S}}_z^2\rangle,$$

$$\sigma_{S_2} = \sqrt{\sigma_x^2 + \sigma_y^2 + \sigma_z^2} = \sqrt{3}(\hbar/2).$$

ПТФ-2.з1. Блоховское представление двухуровневой системы

1) Покажите, что матрицу плотности произвольной двухуровневой системы самого общего вида можно разложить по матрицам Паули в следующем виде:

$$\hat{\rho} = \frac{1}{2}(\hat{\mathbb{I}} + \hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})$$

где $\boldsymbol{n}$ – какой-то вектор. При каком условии на $\boldsymbol{n}$ это корректная матрица плотности?
2) При каком условии на $\boldsymbol{n}$, эта матрица плотности описывает чистое состояние?
3) Вычислите средние значения $\langle\hat{\sigma}_{x,y,z}\rangle$ по состоянию, описываемому такой матрицей плотности.

Solution.

Пусть с вероятностью p_α система может быть приготовлена в состоянии $|\alpha\rangle$. Тогда для такого усреднения мы можем записать:

$$\langle\hat{O}\rangle = \sum_\alpha p_\alpha\langle\alpha|\hat{O}|\alpha\rangle = \mathrm{Tr}(|\alpha\rangle p_\alpha\langle\alpha|\hat{O}) \equiv \mathrm{Tr}(\hat{\rho}\hat{O})$$

Матрица плотности:

$$\hat{\rho} = \sum_{\alpha} p_\alpha |\alpha\rangle\langle\alpha|$$

Матрица плотности – эрмитов оператор $\hat{\rho} = \hat{\rho}^\dagger$ с нормировкой $\mathrm{Tr}\hat{\rho} = \sum\limits_{\alpha} p_\alpha = 1$.

Удобно диагонализовать матрицу плотности (любая эрмитова матрица диагонализуема с вещественными собственными числами λ_n):

$$\hat{\rho}|n\rangle = \lambda_n |n\rangle,$$

$$\mathrm{Tr}\hat{\rho} = \sum_n \lambda_n = 1$$

Матрица плотности неотрицательно определена:

$$\langle\psi|\hat{\rho}|\psi\rangle = \sum_\alpha p_\alpha \langle\psi|\alpha\rangle\langle\alpha|\psi\rangle = \sum_\alpha p_\alpha \langle\psi|\alpha\rangle\langle\alpha|\psi\rangle = \sum_\alpha p_\alpha |\langle\alpha|\psi\rangle|^2 \geq 0$$

Следовательно, все $\lambda_n \geq 0$. А поскольку $\sum\limits_n \lambda_n = 1$, то все $\lambda_n \in [0,1]$. Собственные числа λ_n являются вероятностями оказаться в состоянии $|n\rangle$.

• Матрицы Паули совместно с единичной матрицей $\sigma^0 = \hat{\mathbb{I}}_{2\times 2}$ представляют собой базис в пространстве эрмитовых матриц 2×2 (см. упр. 3 недели 1). Поскольку $\mathrm{Tr}\hat{\rho} = 1$ и $\mathrm{Tr}\sigma_i = 0$, то коэффициент перед $\mathbb{I}$ равен $\frac{1}{2}$:

$$\hat{\rho} = \frac{1}{2}(\hat{\mathbb{I}} + \hat{\vec{\sigma}} \cdot \vec{n}) = \frac{1}{2}\begin{pmatrix} 1+n_z & n_x - in_y \\ n_x + in_y & 1-n_z \end{pmatrix}$$

$$\det\hat{\rho} = \frac{1}{2}(1 - n_z^2 - n_x^2 - n_y^2) = \frac{1}{2}(1 - \boldsymbol{n}^2)$$

$$\det\hat{\rho} = \prod_n \lambda_n \geq 0 \to |\boldsymbol{n}| \leq 1$$

Таким образом, конец вектора $\boldsymbol{n}$ лежит в шаре радиуса 1.

• Квантовая система, описываемая какой-то волновой функцией $|\psi\rangle$ (с вероятностью $p = 1$) можно описать на языке матрицы плотности

$$\hat{\rho} = |\psi\rangle\langle\psi|$$

Состояние, описываемое такой матрицей плотности, носит название *чистого*. В противном случае состояние называется *смешанным*.

Матрица плотности чистого состояния является проектором:

$$\hat{\rho}^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \hat{\rho}$$

$$\mathrm{Tr}\hat{\rho}^2 = \mathrm{Tr}\hat{\rho} = 1$$

В общем случае

$$\mathrm{Tr}\hat{\rho}^2 = \sum_\alpha p_\alpha^2 \leq \sum_\alpha p_\alpha = \mathrm{Tr}\hat{\rho} = 1$$

В случае чистого состояния одно из собственных значений равно 1, остальные равны 0.

$$\det\hat{\rho} = \frac{1}{2}(1 - |\boldsymbol{n}|^2) = 0 \to |\boldsymbol{n}| = 1$$

Таким образом, конец вектора $\boldsymbol{n}$ лежит на сфере радиуса 1.

• Среднее значение по состоянию:

$$\langle\sigma_i\rangle = \mathrm{Tr}(\rho\sigma_i) = \frac{1}{2}\mathrm{Tr}(\hat{\sigma}_i + \hat{\sigma}_i{}^2 n_i) = n_i$$

$$\langle\sigma_{x,y,z}\rangle = n_{x,y,z}$$

Solution..

Суть решения в скучных проверках свойств. (???)
Так как матрица плотности двухуровневой системы имеет размерность 2×2, то ее можно всегда разложить по базису в пространстве матриц 2×2, нужно только проверить, чтобы выполнялись ее свойства.
чтобы $\operatorname{Tr}\hat{\rho} = 1$, необходимо, чтобы был член с единичной матрицей, деленной на 2. эрмитовость очевидна из этого разложения положительно определенность дает на компоненты n условие: $n_1^2+n_2^2+n_3^2 \leqslant 1$

$$\hat{\rho}^2 = \hat{\rho}$$

$$\frac{1}{4}\begin{pmatrix} 1+n_3 & n_1-in_2 \\ n_1+in_2 & 1-n_3 \end{pmatrix}^2 = \frac{1}{2}\begin{pmatrix} 1+n_3 & n_1-in_2 \\ n_1+in_2 & 1-n_3 \end{pmatrix}$$

$$((1+n_3)^2+n_1^2+n_2^2)/2 = 1+n_3, \qquad ((1-n_3)^2+n_1^2+n_2^2)/2 = 1-n_3$$

Теперь посчитаем $\langle\hat{\sigma}_{x,y,z}\rangle$:

$$\langle\hat{\sigma}_x\rangle = \operatorname{Tr}(\hat{\rho}\hat{\sigma}_x) = \frac{1}{2}\operatorname{Tr}\begin{pmatrix} n_1-in_2 & 1+n_3 \\ 1-n_3 & n_1+in_2 \end{pmatrix} = \frac{n_1^2+n_2^2}{2},$$
$$\langle\hat{\sigma}_y\rangle = \frac{i}{2}\operatorname{Tr}\begin{pmatrix} n_1-in_2 & -1-n_3 \\ 1-n_3 & -n_1-in_2 \end{pmatrix} = \frac{-n_1^2-n_2^2}{2},$$
$$\langle\hat{\sigma}_z\rangle = \frac{1}{2}\operatorname{Tr}\begin{pmatrix} 1+n_3 & -n_1+in_2 \\ n_1+in_2 & -1+n_3 \end{pmatrix} = \frac{n_3^2-1}{2}$$

ПТФ-2.з2. Термодинамика двухуровневой системы

Двухуровневая система описывается гамильтонианом $\hat{H} = -\boldsymbol{h}\cdot\hat{\boldsymbol{\sigma}}$, где $\boldsymbol{h} = (h_x, h_y, h_z)$, и находится при температуре T. Вычислите средние значения $\hat{\sigma}_{x,y,z}$.

Solution.

Гиббсовский (канонический) ансамбль:

$$\hat{\rho} = \frac{1}{Z}e^{-\beta\hat{H}}, \quad Z = \operatorname{Tr}(e^{-\beta\hat{H}}) = \operatorname{Tr}(e^{\beta\vec{h}\cdot\hat{\vec{\sigma}}})$$

Воспользуемся упр. 3, п. 3 семинара 1 (там был случай $h = 1$, но он очевидным образом обобщается на случай $h \neq 1$):

$$e^{\beta\boldsymbol{h}\cdot\hat{\boldsymbol{\sigma}}} = \mathbb{I}\cosh\beta h + \frac{\sinh\beta h}{h}\boldsymbol{h}\cdot\hat{\boldsymbol{\sigma}}$$

$$Z = \operatorname{Tr}\left(\mathbb{I}\cosh\beta h + \frac{\sinh\beta h}{h}\boldsymbol{h}\cdot\hat{\boldsymbol{\sigma}}\right) = 2\cosh\beta h$$

$$\hat{\rho} = \frac{\mathbb{I}\cosh\beta h + \frac{\sinh\beta h}{h}\boldsymbol{h}\cdot\hat{\boldsymbol{\sigma}}}{2\cosh\beta h} = \frac{1}{2}\mathbb{I} + \frac{1}{2h}\boldsymbol{h}\cdot\hat{\boldsymbol{\sigma}}\tanh\beta h = \frac{1}{2}\begin{pmatrix} 1+\frac{h_z}{h}\tanh\beta h & \frac{h_x-ih_y}{h}\tanh\beta h \\ \frac{h_x+ih_y}{h}\tanh\beta h & 1+\frac{h_z}{h}\tanh\beta h \end{pmatrix}$$

$$\langle\hat{\sigma}_\alpha\rangle = \operatorname{Tr}(\hat{\rho}\sigma_\alpha) = \frac{1}{2}\operatorname{Tr}\left(\hat{\sigma}_\alpha + \frac{h_\alpha\tanh\beta h}{h}\mathbb{I}\right) = \frac{h_\alpha}{h}\tanh\beta h$$

$$\langle\hat{\sigma}_x\rangle = \frac{h_x}{h}\tanh\beta h, \quad \langle\hat{\sigma}_y\rangle = \frac{h_y}{h}\tanh\beta h, \quad \langle\hat{\sigma}_z\rangle = \frac{h_z}{h}\tanh\beta h$$

Solution..

Вероятность состояний определяется распределением Гиббса, т.е. матрицу плотности можно найти так:

$$\hat{\rho} = \frac{1}{Z}e^{-\beta\hat{H}}, \quad Z = \operatorname{Tr}\left(e^{-\hat{H}/T}\right) = \sum_n e^{-E_n/T}$$

$$E_{1,2} = \pm\sqrt{h_1^2+h_2^2+h_3^2}$$

$$Z = e^{\sqrt{h_1^2+h_2^2+h_3^2}/T} + e^{-\sqrt{h_1^2+h_2^2+h_3^2}/T}$$

$$\begin{aligned} e^{-\hat{H}/T} = e^{i\boldsymbol{h}\cdot\hat{\boldsymbol{\sigma}}/iT} &= I\cos(i\cdot(-1/T)) + i(\boldsymbol{h}\cdot\vec{\sigma})\sin(i\cdot(-1/T)) = I\,\mathrm{ch}(-1/T) - (\boldsymbol{h}\cdot\vec{\sigma})\,\mathrm{sh}(-1/T) = \\ &= \begin{pmatrix} \mathrm{ch}(-1/T) & 0 \\ 0 & \mathrm{ch}(-1/T) \end{pmatrix} - \mathrm{sh}(-1/T)\begin{pmatrix} h_3 & h_1 - ih_2 \\ h_1 + ih_2 & h_3 \end{pmatrix} = \\ &= \begin{pmatrix} -\mathrm{sh}(-1/T)h_3 + \mathrm{ch}(-1/T) & -\mathrm{sh}(-1/T)(h_1 - ih_2) \\ -\mathrm{sh}(-1/T)(h_1 + ih_2) & -\mathrm{sh}(-1/T)h_3 + \mathrm{ch}(-1/T) \end{pmatrix} \end{aligned}$$

Теперь можем считать среднее по $\langle\hat{\sigma}_i\rangle = \mathrm{Tr}\,(\hat{\rho}\hat{\sigma}_i)$:

$$\begin{aligned} \langle\hat{\sigma}_x\rangle &= \frac{1}{Z}\,\mathrm{Tr}\begin{pmatrix} -\mathrm{sh}(-1/T)(h_1 - ih_2) & -\mathrm{sh}(-1/T)h_3 + \mathrm{ch}(-1/T) \\ -\mathrm{sh}(-1/T)h_3 + \mathrm{ch}(-1/T) & -\mathrm{sh}(-1/T)(h_1 + ih_2) \end{pmatrix} = \frac{-2\,\mathrm{sh}(-1/T)h_1}{Z}, \\ \langle\hat{\sigma}_y\rangle &= \frac{i}{Z}\,\mathrm{Tr}\begin{pmatrix} -\mathrm{sh}(-1/T)(h_1 - ih_2) & \mathrm{sh}(-1/T)h_3 - \mathrm{ch}(-1/T) \\ -\mathrm{sh}(-1/T)h_3 + \mathrm{ch}(-1/T) & \mathrm{sh}(-1/T)(h_1 + ih_2) \end{pmatrix} = \frac{2i\,\mathrm{sh}(-1/T)h_2}{Z}, \\ \langle\hat{\sigma}_z\rangle &= \frac{1}{Z}\,\mathrm{Tr}\begin{pmatrix} -\mathrm{sh}(-1/T)h_3 + \mathrm{ch}(-1/T) & \mathrm{sh}(-1/T)(h_1 - ih_2) \\ -\mathrm{sh}(-1/T)(h_1 + ih_2) & \mathrm{sh}(-1/T)h_3 - \mathrm{ch}(-1/T) \end{pmatrix} = 0. \end{aligned}$$

ВШЭ-2024.кр.4а Матрица плотности спина после измерения

Спин-1/2 приготовлен в состоянии $\frac{1}{\sqrt{3}}|\uparrow\rangle + \frac{1+i}{\sqrt{3}}|\downarrow\rangle$. Измеряется проекция спина на ось y. Какие значения могут получиться и с какой вероятностью? Найдите матрицу плотности спина после измерения в базисе $|\uparrow\rangle, |\downarrow\rangle$.

Solution.

В общем случае можно получить формулу для проектора вдоль произвольного направления (в качестве упражнения проделайте, исходя из того, что $|n_\uparrow\rangle = \left(\cos\frac{\theta}{2}e^{-i\varphi/2}\sin\frac{\theta}{2}e^{i\varphi/2}\right)$ и $|n_\downarrow\rangle = \left(-\sin\frac{\theta}{2}e^{-i\varphi/2}\cos\frac{\theta}{2}e^{i\varphi/2}\right)$)

$$\mathbb{P}_n = \begin{pmatrix} \frac{1+n_z}{2} & \frac{n_x - in_p}{2} \\ \frac{n_z + in_y}{2} & \frac{1-n_z}{2} \end{pmatrix},$$

где (n_x, n_y, n_z) являются компонентами вектора Блоха. По условию задачи мы проводим измерения вдоль оси y, т.е. в таком случае вектор Блоха $(0, 1, 0)$ направлен вдоль оси y. Тогда проекторы "вверх"и "вниз"

$$\begin{aligned} \mathbb{P}_{y\downarrow} &= \begin{pmatrix} \frac{1}{2} & -\frac{i}{2} \\ \frac{i}{2} & \frac{1}{2} \end{pmatrix}, \\ \mathbb{P}_{y\downarrow} &= \begin{pmatrix} \frac{1}{2} & \frac{i}{2} \\ -\frac{i}{2} & \frac{1}{2} \end{pmatrix}. \end{aligned}$$

Также нам по условию дан спин- 1/2, которому будет соответствовать следующая матрица плотности

$$\rho_i = \frac{1}{3}\begin{pmatrix} 1 & 1-i \\ 1+i & 2 \end{pmatrix}.$$

Матрца плотности после измерения будет классической смесью двух проекций вдоль двух возможный состояний

$$\begin{aligned} \rho_f &= \mathbb{P}_{y\uparrow}\rho_i\mathbb{P}_{y\dagger} + \mathbb{P}_{y\downarrow}\rho_i\mathbb{P}_{y\downarrow} \\ &= \frac{1}{12}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} + \frac{5}{12}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2} & -\frac{i}{3} \\ \frac{i}{3} & \frac{1}{2} \end{pmatrix} \end{aligned}$$

Вероятность найти спин вдоль оси (или против оси) определяется квадратом скалярного произведения волновых векторов $|\langle y\uparrow|\psi_0\rangle|^2$ (или $|\langle y\downarrow|\psi_0\rangle|^2$), что может быть выражено на языке проектора как

$$\{\text{ вероятность }\} = \langle\psi_0|\,\mathbb{P}_n\,|\psi_0\rangle\,.$$

$$\{\text{ вероятность "вверх" }\} = \langle\psi_0|\,\mathbb{P}_{y\dagger}\,|\psi_0\rangle = \frac{1}{6}$$

$$\{\text{ вероятность "вниз" }\} = \langle\psi_0|\,\mathbb{P}_{y\downarrow}\,|\psi_0\rangle = \frac{5}{6}$$

ВШЭ-2024.кр.4б Матрица плотности спина после измерения

Спин-1/2 приготовили в состоянии вспин вверх». После этого произвели измерение его y-компоненты, затем x-, а затем z-комноненты. Какова матрица плотности спина в конечном состоянии?

Solution.

(сделать по аналогии с прошлой)

ВШЭ-2024.кр.3. Кубит с флуктуирующим напряжением от детектора

В зарядовом кубите (двхуровневой квантовой системе) расстояние межцу уровнями $|0\rangle$ и $|1\rangle$, равное QV_0, определяется поданным затворным напряжением ным напряжением V_0 (коэффициент Q задаётся ёмкостными параметрами кубита). Запишите гамильтониан кубита в базисе $|0\rangle, |1\rangle$.

Дтя измерения состояния кубита к нему подсоединяют квантовый детектор, создающий в процессе работы флуктуирующее напряжение δV, со спектром $\left\langle \delta V_\omega^2 \right\rangle = A\theta(\omega)/\left(\Gamma^2 + \omega^2\right)$. Из-за неидеальности детектора при этом создаётся небольшой матричный элемент перехода между уровнями, равный $q\delta$ V. Найдите зависимость от времени вероятности обнаружить кубит в возбуждённом состоянии $|1\rangle$, если в начальный момент она равна 1.

Solution.

(черт его знает, как эту решать, вроде выше есть похожая задача)

ПТФ-2.з3.* Квантовый парадокс Зенона (30 б).

Рассмотрите двухуровневую систему, описываемую следующим гамильтонианом:

$$\hat{H} = \begin{pmatrix} E_0 & -\Delta \\ -\Delta & E_0 \end{pmatrix}$$

В начальный момент система приготовлена в состоянии $|\psi(0)\rangle = |\uparrow\rangle$. Если бы мы позволили системе эволюционировать самой по себе, то она бы совершала осцилляции Раби; в частности, через время $T = \frac{\pi\hbar}{2\Delta}$ мы бы обнаружили её в состоянии $|\downarrow\rangle$ с вероятностью $P_\downarrow(T) = 1$. Однако теперь вместо этого через каждый промежуток времени $\tau \ll T$ мы проводим измерение наблюдаемой $\hat{\sigma}^z$. Определите вероятность $P_\downarrow(T)$ в таком случае.

Solution.

(??? что делаем???)

$$|\psi(0)\rangle = |\uparrow\rangle$$

$$\hat{\rho}(0) = |\psi(0)\rangle\langle\psi(0)| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\hat{U}(t) = \exp\left(-\frac{i\hat{H}t}{\hbar}\right) = \exp\left(\frac{it}{\hbar}(\Delta\hat{\sigma}_x - E_0\hat{\mathbb{I}})\right) = \exp\left(\frac{it}{\hbar}\Delta\hat{\sigma}_x\right)\exp\left(-\frac{it}{\hbar}E_0\right)$$

$\exp\left(\frac{it}{\hbar}\Delta\hat{\sigma}_x\right) = \hat{\mathbb{I}}\cos\frac{\Delta t}{\hbar} + i\hat{\sigma}_x\sin\frac{\Delta t}{\hbar}$

$$\hat{U}(t) = \begin{pmatrix} \cos\frac{\Delta t}{\hbar} & i\sin\frac{\Delta t}{\hbar} \\ i\sin\frac{\Delta t}{\hbar} & \cos\frac{\Delta t}{\hbar} \end{pmatrix}\exp\left(-\frac{it}{\hbar}E_0\right)$$

Теперь можем записать состояние в любое время:

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle, \quad \langle\psi(t)| = \langle\psi(0)|\hat{U}^\dagger(t)$$

$$\hat{\rho}(t) = \hat{U}(t)|\psi(0)\rangle\langle\psi(0)|\hat{U}^\dagger(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t) =$$
$$= \begin{pmatrix} \cos\frac{\Delta t}{\hbar} & i\sin\frac{\Delta t}{\hbar} \\ i\sin\frac{\Delta t}{\hbar} & \cos\frac{\Delta t}{\hbar} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \cos\frac{\Delta t}{\hbar} & -i\sin\frac{\Delta t}{\hbar} \\ -i\sin\frac{\Delta t}{\hbar} & \cos\frac{\Delta t}{\hbar} \end{pmatrix} = \begin{pmatrix} \cos^2\frac{\Delta t}{\hbar} & -\frac{i}{2}\sin\frac{2\Delta t}{\hbar} \\ \frac{i}{2}\sin\frac{2\Delta t}{\hbar} & \sin^2\frac{\Delta t}{\hbar} \end{pmatrix}$$

После измерения происходит редукция фон-Неймана, приводящая к дефазировке:

$$\hat{\rho}(\tau) = \begin{pmatrix} \cos^2 \frac{\Delta\tau}{\hbar} & 0 \\ 0 & \sin^2 \frac{\Delta\tau}{\hbar} \end{pmatrix}$$

Вероятность направлений спина после 1 измерения:

$$P_\uparrow(\tau) = \rho_{11} = \cos^2 \frac{\Delta\tau}{\hbar}, \quad P_\downarrow(\tau) = \rho_{22} = \sin^2 \frac{\Delta\tau}{\hbar}$$

Те же вероятности были получены в разделе 1.4 без матрицы плотности. Найдём марицу плотности $\hat{\rho}(n\tau)$ через $\hat{\rho}((n-1)\tau)$.

$$\hat{U}(\tau)\hat{\rho}((n-1)\tau)\hat{U}^\dagger(\tau) = \begin{pmatrix} \cos \frac{\Delta t}{\hbar} & i \sin \frac{\Delta t}{\hbar} \\ i \sin \frac{\Delta t}{\hbar} & \cos \frac{\Delta t}{\hbar} \end{pmatrix} \begin{pmatrix} P_\uparrow((n-1)\tau) & 0 \\ 0 & P_\downarrow((n-1)\tau) \end{pmatrix} \begin{pmatrix} \cos \frac{\Delta t}{\hbar} & -i \sin \frac{\Delta t}{\hbar} \\ -i \sin \frac{\Delta t}{\hbar} & \cos \frac{\Delta t}{\hbar} \end{pmatrix} =$$
$$= \begin{pmatrix} P_\uparrow((n-1)\tau) \cos^2 \frac{\Delta t}{\hbar} + P_\downarrow((n-1)\tau) \sin^2 \frac{\Delta t}{\hbar} & -\frac{i}{2}(P_\uparrow((n-1)\tau) - P_\downarrow((n-1)\tau)) \sin \frac{2\Delta t}{\hbar} \\ \frac{i}{2}(P_\uparrow((n-1)\tau) - P_\downarrow((n-1)\tau)) \sin \frac{2\Delta t}{\hbar} & P_\uparrow((n-1)\tau) \sin^2 \frac{\Delta t}{\hbar} + P_\downarrow((n-1)\tau) \cos^2 \frac{\Delta t}{\hbar} \end{pmatrix}$$

После дефазировки:

$$\hat{\rho}(n\tau) = \begin{pmatrix} P_\uparrow((n-1)\tau) \cos^2 \frac{\Delta t}{\hbar} + P_\downarrow((n-1)\tau) \sin^2 \frac{\Delta t}{\hbar} & 0 \\ 0 & P_\uparrow((n-1)\tau) \sin^2 \frac{\Delta t}{\hbar} + P_\downarrow((n-1)\tau) \cos^2 \frac{\Delta t}{\hbar} \end{pmatrix}$$

Вероятность направлений спина после n измерений:

$$P_\uparrow(n\tau) = P_\downarrow((n-1)\tau) \sin^2 \frac{\Delta\tau}{\hbar} + P_\uparrow((n-1)\tau) \cos^2 \frac{\Delta\tau}{\hbar}$$

$$P_\downarrow(n\tau) = P_\downarrow((n-1)\tau) \cos^2 \frac{\Delta\tau}{\hbar} + P_\uparrow((n-1)\tau) \sin^2 \frac{\Delta\tau}{\hbar}$$

Таким образом, нужно решить векторное рекуррентное уравнение (или, что эквивалентно, систему уравнений):

$$\begin{pmatrix} P_\uparrow(n\tau) \\ P_\downarrow(n\tau) \end{pmatrix} = \begin{pmatrix} \cos^2 \frac{\Delta\tau}{\hbar} & \sin^2 \frac{\Delta\tau}{\hbar} \\ \sin^2 \frac{\Delta\tau}{\hbar} & \cos^2 \frac{\Delta\tau}{\hbar} \end{pmatrix} \begin{pmatrix} P_\uparrow((n-1)\tau) \\ P_\downarrow((n-1)\tau) \end{pmatrix}, \quad \begin{pmatrix} P_\uparrow(0) \\ P_\downarrow(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Решение этого уравнения:

$$\begin{pmatrix} P_\uparrow(n\tau) \\ P_\downarrow(n\tau) \end{pmatrix} = \begin{pmatrix} \cos^2 \frac{\Delta\tau}{\hbar} & \sin^2 \frac{\Delta\tau}{\hbar} \\ \sin^2 \frac{\Delta\tau}{\hbar} & \cos^2 \frac{\Delta\tau}{\hbar} \end{pmatrix}^n \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Диагонализуем матрицу:

$$\begin{pmatrix} \cos^2 \frac{\Delta\tau}{\hbar} & \sin^2 \frac{\Delta\tau}{\hbar} \\ \sin^2 \frac{\Delta\tau}{\hbar} & \cos^2 \frac{\Delta\tau}{\hbar} \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \cos \frac{2\Delta\tau}{\hbar} \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

$$\begin{pmatrix} \cos^2 \frac{\Delta\tau}{\hbar} & \sin^2 \frac{\Delta\tau}{\hbar} \\ \sin^2 \frac{\Delta\tau}{\hbar} & \cos^2 \frac{\Delta\tau}{\hbar} \end{pmatrix}^n = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \cos^n \frac{2\Delta\tau}{\hbar} \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 + \cos^n \frac{2\Delta\tau}{\hbar} & 1 - \cos^n \frac{2\Delta\tau}{\hbar} \\ 1 - \cos^n \frac{2\Delta\tau}{\hbar} & 1 + \cos^n \frac{2\Delta\tau}{\hbar} \end{pmatrix}$$

$$\begin{pmatrix} P_\uparrow(n\tau) \\ P_\downarrow(n\tau) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 + \cos^n \frac{2\Delta\tau}{\hbar} & 1 - \cos^n \frac{2\Delta\tau}{\hbar} \\ 1 - \cos^n \frac{2\Delta\tau}{\hbar} & 1 + \cos^n \frac{2\Delta\tau}{\hbar} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 + \cos^n \frac{2\Delta\tau}{\hbar} \\ 1 - \cos^n \frac{2\Delta\tau}{\hbar} \end{pmatrix}$$

Учитывая, что $T = n\tau$, получим

$$P_\downarrow(T) = \frac{1}{2} \left(1 - \cos^{\frac{T}{\tau}} \frac{2\Delta\tau}{\hbar} \right)$$

По формуле Тейлора до 2 порядка:

$$P_\downarrow(T) = \frac{\Delta^2}{\hbar^2} T\tau$$

Выводы и применения парадокса (???)

(пока не знаю.)

ПТФ-2.з4.* Флуктуации магнитного поля и спин (30 б).

Спин-1/2 находится в магнитном поле, направленном вдоль оси z:

$$\hat{H} = -B\hat{\sigma}^z$$

В результате взаимодействия с окружающей средой, магнитное поле испытывает случайные флуктуации: $B \equiv B_0 + \delta B(t)$, которые мы предполагаем гауссовыми с нулевым средним и $\langle \delta B(t)\delta B(t')\rangle = \Gamma\delta(t-t')$. Пусть в начальный момент времени, матрица плотности была самого общего вида:

$$\hat{\rho}(0) = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix}$$

Определите зависимость усреднённой по таким флуктуациям матрицы плотности от времени $\langle\hat{\rho}(t)\rangle$.

Указание: для средних типа $\langle \exp\left(i\int\limits_{t_1}^{t_2}\delta B(t)dt\right)\rangle$ есть следующие два способа:

• Воспользоваться теоремой Вика, из которой следует, что для любой гауссовой величины с нулевым средним выполнено $\langle e^A\rangle = e^{\frac{1}{2}\langle A^2\rangle}$.

• Дискретизовать время, разбив на маленькие участки $t \in (n\delta t, (n+1)\delta t)$ и предположив $\delta B_n = \text{const}$; тогда такой локальный по времени коррелятор эквивалентен $\langle \delta B_n \delta B_m\rangle = \delta_{nm}\frac{\Gamma}{\delta t}$. В результате вы получите дискретное Гауссово распределение, с которым вы уже умеете работать.

Solution.

Уравнение Гейзенберга для эволюции матрицы плотности $\hat{\rho}(t)$:

$$\frac{\partial\hat{\rho}(t)}{\partial t} = \frac{i}{\hbar}[\hat{\rho}(t), \hat{H}(t)] = -\frac{iB(t)}{\hbar}[\hat{\rho}(t), \hat{\sigma}^z]$$

$$[\hat{\rho}(t),\hat{\sigma}^z] = \left[\begin{pmatrix}\rho_{11}(t) & \rho_{12}(t)\\ \rho_{21}(t) & \rho_{22}(t)\end{pmatrix}, \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right] = \begin{pmatrix}\rho_{11}(t) & -\rho_{12}(t)\\ \rho_{21}(t) & -\rho_{22}(t)\end{pmatrix} - \begin{pmatrix}\rho_{11}(t) & \rho_{12}(t)\\ -\rho_{21}(t) & -\rho_{22}(t)\end{pmatrix} = \begin{pmatrix}0 & 2\rho_{12}(t)\\ -2\rho_{21}(t) & 0\end{pmatrix}$$

$$\frac{\partial\hat{\rho}(t)}{\partial t} = \frac{iB(t)}{\hbar}\begin{pmatrix}0 & 2\rho_{12}(t)\\ -2\rho_{21}(t) & 0\end{pmatrix}$$

$$\hat{\rho}(t) = \begin{pmatrix} \hat{\rho}_{11}(t_0) & \hat{\rho}_{12}(t_0)\exp\left(\frac{2i}{\hbar}\int\limits_{t_0}^{t}B(t')dt'\right)\\ \hat{\rho}_{21}(t_0)\exp\left(-\frac{2i}{\hbar}\int\limits_{t_0}^{t}B(t')dt'\right) & \hat{\rho}_{22}(t_0)\end{pmatrix} =$$

$$= \begin{pmatrix} \hat{\rho}_{11}(t_0) & \hat{\rho}_{12}(t_0)\exp\left(\frac{2i}{\hbar}B_0(t-t_0)\right)\exp\left(\frac{2i}{\hbar}\int\limits_{t_0}^{t}\delta B(t')dt'\right)\\ \hat{\rho}_{21}(t_0)\exp\left(-\frac{2i}{\hbar}B_0(t-t_0)\right)\exp\left(-\frac{2i}{\hbar}\int\limits_{t_0}^{t}\delta B(t')dt'\right) & \hat{\rho}_{22}(t_0)\end{pmatrix}$$

Теперь усредним матрицу плотности $\hat{\rho}$ по случайным флуктуациям с помощью теоремы Вика:

$$\left\langle \exp\left(\frac{2i}{\hbar}\int\limits_{t_0}^{t}\delta B(t')dt'\right)\right\rangle = \exp\left(-\frac{2}{\hbar^2}\left\langle\left(\int\limits_{t_0}^{t}\delta B(t')dt'\right)^2\right\rangle\right) =$$

$$= \exp\left(-\frac{2}{\hbar^2}\left\langle\int\limits_{t_0}^{t}\delta B(t')dt'\int\limits_{t_0}^{t}\delta B(t'')dt''\right\rangle\right) = \exp\left(-\frac{2}{\hbar^2}\int\limits_{t_0}^{t}\int\limits_{t_0}^{t}\langle\delta B(t')\delta B(t'')\rangle dt'dt''\right) =$$

$$= \exp\left(-\frac{2}{\hbar^2}\int\limits_{t_0}^{t}\int\limits_{t_0}^{t}\Gamma\delta(t'-t'')dt'dt''\right) = \exp\left(-\frac{2\Gamma}{\hbar^2}\int\limits_{t_0}^{t}dt''\right) = \exp\left(-\frac{2\Gamma}{\hbar^2}(t-t_0)\right)$$

$$\langle\hat{\rho}(t)\rangle = \begin{pmatrix}\hat{\rho}_{11}(t_0) & \hat{\rho}_{12}(t_0)\exp\left(\frac{2(iB_0\hbar-\Gamma)}{\hbar^2}(t-t_0)\right)\\ \hat{\rho}_{21}(t_0)\exp\left(-\frac{2(iB_0\hbar-\Gamma)}{\hbar^2}(t-t_0)\right) & \hat{\rho}_{22}(t_0)\end{pmatrix}$$

Теперь сделаем усреднение другим способом, дискретизуем время:

$$\left\langle \exp\left(\frac{2i}{\hbar}\int\limits_{t_0}^{t}\delta B(t')dt'\right)\right\rangle = \left\langle \exp\left(\frac{2i}{\hbar}\sum_{n=1}^{N}\delta B_n\delta t\right)\right\rangle = \left\langle \prod_{n=1}^{N}\exp\left(\frac{2i\delta t}{\hbar}\delta B_n\right)\right\rangle$$

где $N = \frac{t-t_0}{\delta t}$. Разложим каждую экспоненту по формуле Тейлора до 1 порядка:

$$\exp\left(\frac{2i\delta t}{\hbar}\delta B_n\right) = 1 + \frac{2i\delta t}{\hbar}\delta B_n - \frac{2(\delta t)^2}{\hbar^2}(\delta B_n)^2$$

Поскольку δB_n в каждой экспоненте независимы, то

$$\left\langle \prod_{n=1}^{N}\exp\left(\frac{2i\delta t}{\hbar}\delta B_n\right)\right\rangle = \prod_{n=1}^{N}\left\langle \exp\left(\frac{2i\delta t}{\hbar}\delta B_n\right)\right\rangle = \prod_{n=1}^{N}\left\langle 1 + \frac{2i\delta t}{\hbar}\delta B_n - \frac{2(\delta t)^2}{\hbar^2}(\delta B_n)^2\right\rangle =$$

$$= \prod_{n=1}^{N}\left(1 - \frac{2\delta t}{\hbar^2}\Gamma\right) = \prod_{n=1}^{N}\left(1 - \frac{2\Gamma(t-t_0)}{\hbar^2 N}\right)^N$$

Устремим число слагаемых в разбиении $N \to \infty$ и воспользуемся 2 замечательным пределом:

$$\left\langle \prod_{n=1}^{N}\exp\left(\frac{2i\delta t}{\hbar}\delta B_n\right)\right\rangle = \exp\left(-\frac{2\Gamma}{\hbar^2}(t-t_0)\right)$$

Таким образом, получаем тот же ответ:

$$\langle\hat\rho(t)\rangle = \begin{pmatrix} \hat\rho_{11}(t_0) & \hat\rho_{12}(t_0)\exp\left(\frac{2(iB_0\hbar-\Gamma)}{\hbar^2}(t-t_0)\right) \\ \hat\rho_{21}(t_0)\exp\left(-\frac{2(iB_0\hbar-\Gamma)}{\hbar^2}(t-t_0)\right) & \hat\rho_{22}(t_0)\end{pmatrix}$$

(??? допишу потом, качественно в чем наш результат, который мы получили???)

Моя давняя попытка решения (??)

(??????!!)
если $\hat H = -B\cdot\hat\sigma^z$, где B - магнитное поле, которое флуктуирует так, что $\langle\delta B(t)\delta B\,(t')\rangle = \Gamma\delta\,(t-t')$,
Посмотрим, как будет меняться система с

$$\hat\rho(0) = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22}\end{pmatrix}.$$

$$\hat H(t) = -B(t)\cdot\hat\sigma^z = -(B_0+\delta B(t))\hat\sigma^z$$

$$\hat\rho(0) = \begin{pmatrix} -\operatorname{sh}(-1/T)(B_0+\delta B(t)) + \operatorname{ch}(-1/T) & 0 \\ 0 & -\operatorname{sh}(-1/T)(B_0+\delta B(t)) + \operatorname{ch}(-1/T)\end{pmatrix}$$

и дальше я не знаю, что делать.
если отталкиваться от распределения Гиббса, то можно прийти к тому, что подсказывается в задаче.

$$\langle\hat\rho(t)\rangle = \langle e^{-\hat{H(t)}/T}\rangle = \langle e^{i(B_0+\int_{t_1}^{t_2}\delta B(t)dt)\hat\sigma^z)/iT}\rangle = \hat\rho(0)\langle e^{\int_{t_1}^{t_2}\delta B(t)dt\hat\sigma^z/(iT)}\rangle$$

Для подсчета этого воспользуемся следствием теоремы Вика $\langle e^A\rangle = e^{\frac12\langle A^2\rangle}$
Поэтому

$$\langle\hat\rho(t)\rangle = \hat\rho(0)e^{\int_{t_1}^{t_2}\langle\delta B(t)^2\rangle dt\hat\sigma^z/(2iT)} = \hat\rho(0)e^{i\int_{t_1}^{t_2}\Gamma dt\hat\sigma^z/(2iT)} = \hat\rho(0)e^{\Gamma\Delta t/(2T)}$$

(?????? потом подумаю.)

17.2.2 Problems about stationary states in potentials 1

1D колодец (?)

Определить волновую функцию в $U(x) = \begin{cases} -U_0, & |x| < a \\ 0, & |x| > a \end{cases}$

Solution.

Волновую функцию находим, решая уравнение Шредингера в двух областях, энергию находим с помощью k, который квантуется из вида волновой функции и граничных условий.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi = E\psi$$

(???)

$$E_n = \frac{\pi^2\hbar^2}{2ma^2}n^2, \quad n = 1, 2, 3, ...$$

Условие на стационарные состояния можно написать как сравнение характеристик ямы и частицы: (почему?)

$$U_0 a^2 > \frac{\pi^2\hbar^2}{8m}$$

2D циллиндрический колодец

Найти уровни энергии для частицы массы M в двумерном $U(\boldsymbol{r}) = \begin{cases} -U_0, & r < a \\ 0, & r > a \end{cases}$. Рассмотрите предел мелкой ямы.

Solution.

Решаем через функции Бесселя, далее за счет сшивки находим энергию. Для мелкой ямы раскладываем спецфункции до 1-го и следующего порядка и подставляем в условие сшивки.

Запишем уравнение Шрёдингера в цилиндрических координатах $\psi(r, \varphi)$:

$$-\frac{\hbar^2}{2M}\left(\frac{\partial^2\psi}{\partial r^2} + \frac{1}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\varphi^2}\right) + U(r)\psi(r) = E\psi(r)$$

Введём $\varkappa$: $\frac{\hbar^2\varkappa^2}{2M} = -E = |E|$. Подставим $\psi(r, \varphi) = \psi(r)e^{im\varphi}$, получим:

$$\psi''(r) + \frac{1}{r}\psi'(r) - \left(\frac{2MU(r)}{\hbar^2} + \varkappa^2 + \frac{m^2}{r^2}\right)\psi(r) = 0$$

• Вне ямы $U(r) = 0$, введем координату $z = \varkappa r$, получим уравнение:

$$\psi''(z) + \frac{1}{z}\psi'(z) - \left(1 + \frac{m^2}{z^2}\right)\psi(z) = 0.$$

В общем случае двумя линейно-независимыми решениями этого уравнения являются модифицированные функции Бесселя:

$$\psi(z) = A_1 I_m(z) + A_2 K_m(z)$$

Для нашей задачи поиска связанных состояний коэффициент $A_1 \equiv 0$, поскольку волновая функция должна затухать на бесконечности. Значит

$$\psi(r > a) = AK_m(\varkappa r).$$

• Вне ямы $U(r) = U_0$, введём эффективный волновой вектор $k^2 = \frac{2M(U_0 - |E|)}{\hbar^2} = \frac{2MU_0}{\hbar^2} - \varkappa^2$ и сделаем подстановку подстановку $z = kr$. Получаем похожее уравнение, отличающееся лишь знаком единицы (эквивалентно, эти уравнения связаны заменой $z \mapsto iz$):

$$\psi''(z) + \frac{1}{z}\psi'(z) + \left(1 - \frac{m^2}{z^2}\right)\psi(z) = 0$$

В качестве его линейно-независимых решений, как правило, выбирают либо функции Бесселя и Неймана, либо функции Ганкеля:

$$\psi(z) = B_1 J_m(z) + B_2 Y_m(z) = C_1 H_m^{(1)}(z) + C_2 H_m^{(2)}(z)$$

Нас интересует решение, которое в нуле регулярно, поэтому естественный выбор - это функция Бесселя $\psi(x < a) = BJ_m(kr)$.

Для уровней энергии запишем сшивку логарифмической производной $\frac{d}{dz}\ln\psi(a-0) = \frac{d}{dz}\ln\psi(a+0)$:

$$\frac{kaJ'_m(ka)}{J_m(ka)} = \frac{\varkappa a K'_m(\varkappa a)}{K_m(\varkappa a)}$$

Аналитически это уравнение можно решить лишь в разных предельных случаях.

Предел мелкой ямы

Решим это уравнение аналитически в пределе мелкой ямы: $U_0 \ll \frac{\hbar^2}{Ma^2}$. Этот предел соответствует малым $ka \approx \sqrt{\frac{U_0}{\hbar^2/2Ma^2}} \ll 1$ и $\varkappa a = \sqrt{\frac{|E|}{\hbar^2/2Ma^2}} \ll 1$, и мы можем воспользоваться асимптотиками специальных функций.

Основное состояние из общих соображений минимальности энергии должно соответствовать нулевому орбитальному квантовому числу $m = 0$. Чтобы производная не занулилась, нужен следующий член разложения: $J_0(z)|_{z\ll 1} \approx 1 - \frac{z^2}{4}$. Получаем уравнение на сшивку:

$$ka \cdot \left(-\frac{ka}{2}\right) = \frac{\varkappa a\left(-\frac{1}{xa}\right)}{\ln\frac{2e^{-\gamma}}{xa}}$$

получим соотношение

$$\varkappa a = 2e^{-\gamma}\exp\left(-\frac{2}{k^2a^2}\right).$$

Найдем уровни энергии, подставив $\varkappa^2 = \frac{2M|E|}{\hbar^2}$ и принимая, что $k^2|_{|E|\ll 1} \approx \frac{2MU_0}{\hbar^2}$:

$$|E| = C\frac{\hbar^2}{Ma^2}\exp\left(-\frac{2\hbar^2/Ma^2}{U_0}\right),$$

где $C = 2e^{-2\gamma} \approx 0.630$.

Этот ответ в точности совпадает с общим ответом для мелкой ямы даваемый формулой: $|E| = \#\frac{\hbar^2}{Ma^2}\exp\left(-\frac{2\pi\hbar^2}{M}|\int U(\boldsymbol{r})d^2\boldsymbol{r}|^{-1}\right)$, где интеграл $\int U(\boldsymbol{r})d^2\boldsymbol{r} = -U_0\pi a^2$, таким образом, получаем:

$$|E| = \#\frac{\hbar^2}{Ma^2}\exp\left(-\frac{2\hbar^2/Ma^2}{U_0}\right).$$

Однако константу через нее не найти.

ПТФ-3.у2. Прямоугольная яма

Продемонстрируйте, что в случае, когда эта яма — мелкая, точное решение для прямоугольной ямы

$$U(x) = \begin{cases} -U_0, & -\frac{a}{2} \le x \le \frac{a}{2} \\ 0, & \text{otherwise} \end{cases}$$

совпадает с приближённой формулой для мелкой ямы.

Solution.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E - U(x))\psi(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = \begin{cases} E\psi(x), & x \in (-\infty, -\frac{a}{2}) \cup (\frac{a}{2}, \infty) \\ (E+U_0)\psi(x), & -\frac{a}{2} \le x \le \frac{a}{2} \end{cases}$$

$$-U_0 < E < 0$$
$$\kappa^2 := -\frac{2mE}{\hbar^2}, \qquad k^2 := \frac{2m(E+U_0)}{\hbar^2}$$

Поскольку потенциал $U(x)$ – чётная функция, то и гамильтониан $H(x) = \frac{p^2}{2m} + U(x)$ чётный и коммутирует с оператором инверсии. Собственные функции оператора инверсии – чётные и нечётные функции. Будем искать чётные $\psi(x)$. Из $\int\limits_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$ следует, что

$$\psi(x) = \begin{cases} \psi_I(x) = Ae^{\kappa x}, & x < -\frac{a}{2} \\ \psi_{II}(x) = B\cos kx, & -\frac{a}{2} < x < \frac{a}{2} \\ \psi_{III}(x) = Ae^{-\kappa x}, & x > \frac{a}{2} \end{cases}$$

Запишем граничные условия (из чётности достаточно их записать в одной точке $x = \frac{a}{2}$):

$$\psi_{II}\left(\frac{a}{2}\right) = \psi_{III}\left(\frac{a}{2}\right), \quad \psi'_{II}\left(\frac{a}{2}\right) = \psi'_{III}\left(\frac{a}{2}\right)$$

$$Ae^{\frac{-\kappa a}{2}} = B\cos\frac{ka}{2}, \quad -\kappa Ae^{\frac{-\kappa a}{2}} = -\kappa B\sin\frac{ka}{2}$$

$$\tan\frac{ka}{2} = \frac{\kappa}{k} > 0$$

$$\tan\sqrt{\frac{m(E+U_0)}{2}}\frac{a}{\hbar} = \sqrt{-\frac{E}{E+U_0}}$$

В случае мелкой ямы:

$$U_0 \ll \frac{\hbar^2}{ma^2}, \quad |E| < U_0 \ll \frac{\hbar^2}{ma^2}$$

В случае нечётных функций $\tan\frac{ka}{2}$ получился бы отрицательным и условие мелкой ямы выполниться бы не могло. Поскольку $\sqrt{\frac{m(E+U_0)}{2}}\frac{a}{\hbar}$ мало, то и $\sqrt{-\frac{E}{E+U_0}}$ тоже, значит $E \ll U_0$

$$\sqrt{\frac{mU_0}{2}}\frac{a}{\hbar} = \sqrt{-\frac{E}{U_0}}$$

$$E = -\frac{ma^2U_0^2}{2\hbar^2}$$

$$|E_{\text{мелк яма}}| = \frac{m}{2\hbar^2}\left(\int\limits_{-\infty}^{\infty} U(x)dx\right)^2 = \frac{ma^2U_0^2}{2\hbar^2}$$

Формулы совпадают.

Б-2.2.2 1D цилиндрическая яма

Найти уровни энергии и собственные функции частицы в $U(x) = \begin{cases} -U_0, & |x| < a \\ 0, & |x| > a \end{cases}$, используя симметрию потенциала ($U(x) = U(-x)$).

Solution..

Используем оператор инверсии $\hat{I}$. Поскольку в координатном представлении

$$\hat{\mathrm{H}} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x), \qquad \text{а также } U(x) = U(-x),$$

получаем $[\hat{I}, \hat{\mathrm{H}}] = 0$. Таким образом, волновые функции невырожденного дискретного спектра данной задачи ($E < 0$) обладают определенной четностью

$$\begin{cases} \hat{\mathrm{H}}\psi_E(x) = E\psi_E(x), \\ \hat{I}'\psi_E(x) = \pm\psi_E(x), \end{cases}$$

и данная система уравнений будет заведомо совместна. Обозначая

$$\varkappa^2 = \frac{2m}{\hbar^2}|E|, \quad k^2 = k_0^2 - \varkappa^2, \quad k_0^2 = \frac{2mU_0}{\hbar^2},$$

получим уравнения для определения $\psi_E(x)$ при $|x| < a$:

$$\psi''(x) + k^2\psi_E(x) = 0$$

и при $|x| > a$:

$$\psi''(x) - x^2\psi(x) = 0.$$

Таким образом, для четных состояний получаем $\psi_E{}^{(+)}(x) = A\cos kx$ при $|x| < a$ и $\psi_E^{(+)(x)} = Be^{-x|x|}$ при $|x| > a$. Вследствие явного учета четности функции граничное условие достаточно поставить в одной из точек $x = \pm a$. Из условия непрерывности логарифмической производной $\frac{\psi_E'(a+0)}{\psi_E(a+a)} = \frac{\psi_E'(a-0)}{\psi_E(a-0)}$ получим

$$k\operatorname{tg} ka = \varkappa, \quad k^2 = k_0^2 - \varkappa^2, \text{ или } \left(\frac{k_0}{k}\right)^2 = 1 + \operatorname{tg}^2 ka.$$

На основании этого имеем

$$|\cos ka| = \frac{ka}{k_0 a}$$

при обязательном дополнительном условии $\operatorname{tg} ka > 0$, которое следует из (1). Уровни энергии определяются формулой $E_n = -\hbar^2\varkappa_n^2/(2m)$, где $n = 0, 1, 2, \ldots$ (рис. 2.1).

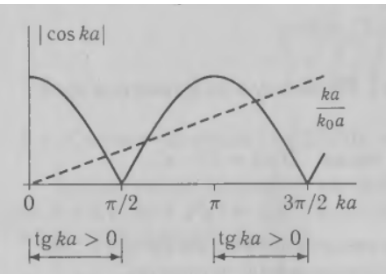


Рис. 2.1. Определение уровней энергии для четных состояний

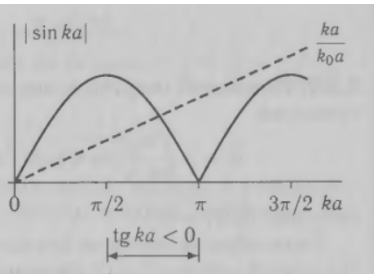


Рис. 2.2. Определение уровней энергии для нечетных состояний

Четное состояние существует при малой глубине U_0 ямы ($k_0 a > 0$). N четных состояний существует при $k_0 a \geqslant (N-1)\pi$. Из условия непрерывности функции

$$\psi(a-0) = \psi(a+0)$$

получаем $B = Ae^{\varkappa a}\cos ka$. Условие нормировки дает

$$1 = 2|A|^2\left(\int_0^a \cos^2 kx dx + \int_a^\infty \cos^2 kae^{-2x(x-a)}dx\right),$$

откуда в результате несложных вычислений имеем

$$A = \frac{1}{\sqrt{a}}\left(1 + \frac{\sin 2ka}{2ka} + \frac{\cos^2 ka}{\varkappa a}\right)^{-1/2}, \quad B = Ae^{\varkappa a}\cos ka.$$

Для нечетных состояний волновая функция должна иметь вид

$$\psi_E^{(-)}(x) = \begin{cases} A\sin kx, & |x| < a, \\ B\operatorname{sign}(x)e^{-x|x|}, & |x| > a. \end{cases}$$

Уровни энергии для нечетных состояний определяются из уравнения $k\operatorname{ctg} ka = -\varkappa$, $k^2 = k_0^2 - \varkappa^2$, Т. е. $\left(\frac{k_0}{k}\right)^2 = 1 + \operatorname{ctg}^2 ka$ или

$$|\sin ka| = \frac{ka}{k_0 a} \quad \text{при } \operatorname{tg} ka < 0.$$

Как видно из рис. 2.2, нечетные дискретные состояния существуют при условии $k_0 a \geqslant \pi/2, (ka/\,(k_0 a) = 1\,,$ когда $k_0 a = \pi/2)$, т. е.

$$U_0 \geqslant \frac{\pi^2}{8}\frac{\hbar^2}{ma^2}.$$

Это и есть условие существования хотя бы одного нечетного состояния в такой яме. N нечетных состояний существует при $k_0 a \geqslant \pi N/2$. Из непрерывности функции $\psi(a+0) = \psi(a-0)$ следует

$$B = Ae^{\varkappa a}\sin ka.$$

Учитываем условие нормировки нашей функции

$$1 = 2|A|^2\left(\int\limits_0^a \sin^2 kx dx + \sin^2 ka\int\limits_a^\infty e^{-2x(x-a)}dx\right)$$

и получаем итоговый результат:

$$A = \frac{1}{\sqrt{a}}\left(1 - \frac{\sin 2ka}{2ka} + \frac{\sin^2 ka}{\varkappa a}\right)^{-1/2}, \quad B = Ae^{\varkappa a}\sin ka.$$

ПТФ-3.2y Мелкая прямоугольная яма (???)

Рассмотрим задачу о частице в прямоугольной яме:

$$U(x) = \begin{cases} -U_0, & -\frac{a}{2} \leq x \leq \frac{a}{2} \\ 0, & \text{otherwise} \end{cases}$$

Продемонстрируйте, что в случае, когда эта яма - мелкая, точное решение совпадает с приближённой формулой для мелкой ямы.

Solution.

(!!! скоро решу, пока просто не особо про нее думал. по идее проблем с решением не должно быть.)

Б-2.2.3 Сила давления на стенку

Используя формулу Фейнмана-Хеллмана $\frac{\partial E_n}{\partial \lambda} = \langle n|\frac{\partial \hat{H}}{\partial \lambda}|n\rangle$, вычислить силу, с которой частица действует на стенку потенциального ящика.

Solution..

Основная идея в том, что мы считаем силу как производную энергии по расстоянию, поэтому формула Фейнмана-Хеллмана как раз сразу и дает ответ.

Сила, действующая на частицу со стороны потенциальной ямы, представляет собой оператор $\hat{\mathrm{F}} = -d\hat{U}/dx = -d\hat{\mathrm{H}}/dx$. Рассмотрим вначале яму конечной глубины U_0, имея в виду дальнейший предельный переход $U_0 \to \infty$. При этом

$$U(x) = U_0(\theta(x-a) + 1 - \theta(x)), \qquad \theta(x) = \begin{cases} 0, & x < 0, \\ 1, & x > 0. \end{cases}$$

Отсюда следует, что

$$\hat{\mathrm{F}} = -\frac{d\hat{\mathrm{U}}}{dx} = U_0(\delta(x) - \delta(x-a)).$$

Используя теорему Фейнмана-Гельмана, находим

$$\langle n|\hat{\mathrm{F}}_{\mathrm{пр}}|n\rangle = \langle n|\frac{\partial\hat{\mathrm{H}}}{\partial a}|n\rangle = \frac{\partial E_n}{\partial a} = -\frac{\pi^2\hbar^2}{ma^3}n^2 = -\frac{2E_n}{a}.$$

Мы нашли среднее значение силы, действующей на частицу со стороны правой стенки потенциального ящика. Сила, которая действует на стенку ящика со стороны частицы, имеет противоположный знак.

Б-2.2.4 Яма рядом со стенкой

Найти уровни энергии и собственные функции частицы в

$$U(x) = \begin{cases} \infty, & x < 0 \\ -U_0, & 0 < x < a \\ 0, & x > a \end{cases}$$

Указать условие существования по крайней мере одного дискретного уровня энергии в такой яме.

Solution..

Можно сразу написать ответ, вспомнив, что если бы не было бесконечной стенки, то были бы известные простые решения, а стенка только дает другую нормировку, потому что с ней другая область пространства свободна для частицы.

(решу заново, без отсылок, это запросто, просто не до нее пока что)

Получим решение задачи о состояниях дискретного спектра в данной потенциальной яме на основании анализа нечетных решений $\psi_E^{(-)}(x)$ задачи 2.2.2. Граничные условия, накладываемые на волновую функцию в точке $x = 0$ и на ψ и ψ' в точке $x = a$, совпадают с соответствующими граничными условиями для $\psi_E^{(-)}(x)$. Однако область, где волновая функция отлична от нуля, уменьшается вдвое. Поэтому $\psi_E^{(-)}(x)$ нужно умножить на $\sqrt{2}$. В итоге получим волновые функции в виде

$$\psi_E(x) = \begin{cases} \sqrt{2}\psi_E^{(-)}(x), & x > 0, \\ 0, & x \leqslant 0. \end{cases}$$

Б-2.2.5 Нахождение вне простой ямы

Пусть в потенциальной яме конечной высоты существует единственный уровень энергии с очень маленькой энергией связи: $|\varepsilon| \ll \hbar^2/\left(2ma^2\right)$ (т. е. $\varkappa := \sqrt{2m|\varepsilon|}/\hbar \ll 1$). Найти вероятность обнаружения частицы вне потенциальной ямы. Можно ли истолковать полученный результат на основе классической механики?

Solution..

Будем считать, что яма мелкая, и тогда, как это следует из анализа задачи о такой яме, в ней присутствует единственный дискретный уровень энергии, отвечающий четной волновой функции. Таким образом, $k_0 a \ll 1$, или $\frac{2mU_0}{\hbar^2}a^2 \ll 1$. Обозначим

$$U_0 = \frac{\hbar^2 k_0^2}{2m}, \quad |\varepsilon| = \frac{\hbar^2 \varkappa^2}{2m}, \quad k^2 = k_0^2 - \varkappa^2.$$

Также будем считать, что энергия связи мала по сравнению с глубиной ямы: $|\varepsilon| \ll U_0$, или $\varkappa \ll k_0$. Оказывается, что при этих предположениях также и $ka \ll 1$, и мы решаем приближенно (с учетом малости ka) трансцендентное уравнение для определения значений энергии:

$$(k_0 a)^2 \cos^2 ka = (ka)^2.$$

В результате имеем

$$\varkappa^2 \approx k_0^4 a^2 \equiv \varkappa_0^2.$$

Получается, что значение энергии связи $|\varepsilon| = |\varepsilon_0|$ гораздо меньше глубины ямы (как и ожидалось):

$$|\varepsilon_0| = \frac{\hbar^2 \varkappa_0^2}{2m} = U_0 \left(k_0 a\right)^2 \ll U_0.$$

Волновая функция в этом приближении имеет вид

$$\psi_0(x) \simeq \begin{cases} B_0 e^{-\varkappa_0 |x|}, & |x| > a, \\ A_0 \cos kx, & |x| \leqslant a, \end{cases}$$

причем $A_0 \simeq B_0 = A|_{ka \to 0} = \sqrt{\varkappa_0}$. Вероятность нахождения частицы в пределах ямы при этом

$$W \simeq \varkappa_0 \int\limits_{-a}^{a} \cos^2 kx dx \simeq 2\varkappa_0 a \ll 1,$$

и, как мы убеждаемся, с подавляющей вероятностью ($\simeq 1$) частица будет находиться вне пределов ямы, т. е. в классически недоступной области. Очевидно, что это существенно квантовое явление, и классическая интерпретация для него невозможна.

Кстати, при $a \to 0, U_0 \to \infty$, но при $U_0 a = \text{const}$, пределом данного потенциала является δ-яма, в которой также имеется всего одно четное состояние дискретного спектра:

$$U(x) = -\frac{h^2}{m}\varkappa_0\delta(x) = \lim_{a\to 0}\left[-\frac{\hbar^2\varkappa_0}{2ma}\theta(a-|x|)\right] = \lim_{a\to 0}\left[-U_0\theta(a-|x|)\right].$$

17.2.3 Problems about stationary states in potentials 2

Б-2.2.17 Показатель преломления света по квантовой механике (!??!?!??!)

На плоскость $z = 0$, разделяющую области пространства с потенциалами

$$U = \begin{cases} U_1, & z < 0 \\ U_2, & z > 0 \end{cases}$$

падает снизу волна де-Бройля, направление которой составляет угол θ_1 с осью z. Найти закон преломления и показатели преломления для обеих сред. Найти коэффициенты отражения и прохождения. При каких условиях будет наблюдаться полное внутреннее отражение? Каково при этом поведение волны во второй среде?

Solution.

(??? решу потом, пока не дошел ещё.)
Вначале введем обозначения

$$E - U_1 = \frac{\hbar^2 k^2}{2m} > 0, \quad E - U_2 = \frac{\hbar^2 q^2}{2m} > 0.$$

Таким образом, мы считаем величины k и q действительными.

В полупространстве $z < 0$ (область 1) волновая функция - решение уравнения Шредингера будет иметь вид

$$\psi_1(\mathbf{r}) = e^{i\mathbf{kr}} + Ae^{i\mathbf{k'r}},$$

где A - амплитуда отраженной волны, $\mathbf{k}$ и $\mathbf{k'}$ - волновые векторы падающей и отраженной волны. В полупространстве $z > 0$ (область 2) волновая функция описывает только прошедшую волну

$$\psi_2(\mathbf{r}) = Be^{i\mathbf{qr}}.$$

Здесь q - волновой вектор прошедшей волны. На плоскости $z = 0$ должны выполняться условия

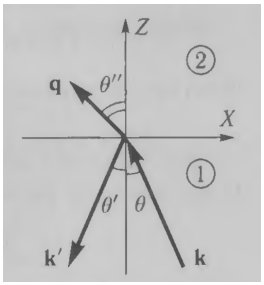
$$\begin{cases} \psi_1(x,y) = \psi_2(x,y), \\ \psi_1'(x,y) = \psi_2'(x,y), \end{cases}$$

откуда следует равенство фаз и амплитуд этих функций. Если направить ось перпендикулярно плоскости падения, то условие равенства фаз запишется совсем просто (рис. 2.7): $k_x x = k'_x x = q_x x$, или $k\sin\theta = k\sin\theta' = q\sin\theta''$, откуда немедленно следует $\theta = \theta'$ (закон отражения) и закон преломления:

$$\frac{\sin\theta''}{\sin\theta} = \frac{q}{k}.$$

По аналогии с оптикой определим показатель преломления:

$$n = \frac{q}{k} = \sqrt{\frac{E-U_2}{E-U_1}}.$$



Это показатель преломления второй "среды» относительно первой. Если же принять $n = 1$ для $U = 0$, то получим показатели преломления обеих «сред» относительно вакуума:

$$n_1 = \sqrt{1 - \frac{U_1}{E}}, \quad n_2 = \sqrt{1 - \frac{U_2}{E}}.$$

Теперь используем условия равенства амплитуд

$$\begin{cases} 1 + A = B, \\ 1 - A = \frac{q_z}{k_z} B. \end{cases}$$

Решаем эту систему и находим коэффициенты прохождения и отражения:

$$D = \frac{|j_z^{\text{прош}}|}{|j_z^{\text{пад}}|} = \frac{q_z}{k_z}|B|^2 = \frac{4q_z k_z}{(k_z + q_z)^2},$$
$$R = \frac{|j_z^{\text{отр}}|}{|j_z^{\text{пад}}|} = |A|^2 = \frac{(k_z - q_z)^2}{(k_z + q_z)^2}.$$

Полное отражение возникает, когда $E < U_2$, и тогда $q = i\varkappa$ - чисто мнимая величина. При этом из равенства (1) следует

$$q_z^2 = q^2 - q_x^2 = -\varkappa^2 - k^2 \sin^2\theta < 0,$$

поэтому и $q_z = i\varkappa_z$ - чисто мнимое. При таких условиях $R = 1$, а плотность потока прошедшей волны равна нулю. Волновая функция в области 2 пропорциональна $e^{-\varkappa_z z}$, т. е. экспоненциально убывает.

ПТФ-3.з4. Регуляризованный кулоновский потенциал (40 б).

Найдите энергию основного состояния в регуляризованном одномерном Кулоновском потенциале $U(x) = -\frac{e^2}{\sqrt{x^2+a^2}}$, считая что регуляризация происходит на масштабах меньше Боровского радиуса $a \ll a_B = \frac{\hbar^2}{me^2}$.

Solution.

$$\bar{U}(p) := \int\limits_{-\infty}^{\infty} U(x) \exp\left(-\frac{ipx}{\hbar}\right) dx = -\int\limits_{-\infty}^{\infty} \frac{e^2 \exp(-\frac{ipx}{\hbar})}{\sqrt{x^2+a^2}} dx$$

В данном случае нельзя приближать выносом $\bar{U}(p)$ за интеграл, ибо $\bar{U}(p)$ меняется быстро ($U(x)$ медленная).

$$-\int\limits_{-\infty}^{\infty} \frac{\bar{U}(p)(dp)}{|E| + \frac{p^2}{2m}} = 1$$

$$\int\limits_{-\infty}^{\infty} \left(\int\limits_{-\infty}^{\infty} \frac{e^2 \exp(-\frac{ipx}{\hbar})}{2\pi\hbar\sqrt{x^2+a^2}(|E| + \frac{p^2}{2m})} dx \right) dp = 1$$

$$\int\limits_{-\infty}^{\infty} \left(\int\limits_{-\infty}^{\infty} \frac{e^2 \exp(-\frac{ipx}{\hbar})}{2\pi\hbar\sqrt{x^2+a^2}(|E| + \frac{p^2}{2m})} dp \right) dx = 1$$

$$\int\limits_{-\infty}^{\infty} \sqrt{\frac{m}{2|E|}} \frac{e^2 \exp(-\frac{\sqrt{2m|E|}|x|}{\hbar})}{\hbar\sqrt{x^2+a^2}} dx = 1$$

$k := a\frac{\sqrt{2m|E|}}{\hbar} = \frac{a}{e}\sqrt{\frac{2|E|}{a_B}}$; $u := \frac{|x|}{a}$, тогда

$$2\int\limits_0^{\infty} \left(\frac{\exp(-ku)}{\sqrt{1+u^2}} \right) du = \frac{ka_B}{a}$$

В пределе малых k экспоненту можно разложить до 1 члена в ряде Тейлора и взять верхний предел $\frac{1}{k}$: (????? не знаю, почему так, но проверил на Вольфраме, действительно примерно выражения совпадают!)

$$\int\limits_0^\infty \left(\frac{\exp(-ku)}{\sqrt{1+u^2}}\right) du \approx \int\limits_0^{1/k} \frac{du}{\sqrt{1+u^2}} = \ln\left[u+\sqrt{1+u^2}\right]\Big|_0^{1/k} = \ln\left(\frac{2}{k}\right)$$

$$2\ln\left(\frac{2}{k}\right) = \frac{ka_B}{a}$$

$$k\exp\left(\frac{ka_B}{2a}\right) = 2$$

$z := \frac{ka_B}{2a}$,

$$\exp(z) = \frac{a_B}{a}\frac{1}{z}$$

$$z^{(0)} = 1$$

$$z^{(1)} = \ln\left(\frac{a_B}{a}\right)$$

$$z = \ln(a_B/a) + \mathcal{O}(\ln\ln(a_B/a)) \qquad \Rightarrow \qquad k \approx \frac{2a\ln(a_B/a)}{a_B}$$

$$E \approx -2\frac{e^2}{a_B}\ln^2\frac{a_B}{a}$$

Еще одно, давнее решение

УШ в импульсной форме, считая $\hbar = 1$, имеет типичное решение

$$\psi(p) = -\frac{1}{p^2/(2m)+|E|}\int\limits_{-\infty}^{\infty}\frac{U_{p-p'}dp'}{2\pi}\psi(p'),$$

где $U_{p-p'} = -\int U(x)e^{-i(p-p')x}dx = -\int \frac{aU_0}{a+|x|}\cos((p-p')x)dx$.

То есть решаем задачу о нахождении E из уравнения:

$$\psi(p) = -\frac{1}{2\pi(p^2/(2m)+|E|)}\int\limits_{-\infty}^{\infty}\int\frac{-aU_0}{a+|x|}e^{-i(p-p')x})dx\psi(p')dp'$$

Преобразуем

$$\int\limits_{-\infty}^{\infty}\psi(p')dp' = -\frac{U_p}{p^2/(2m)+|E|}\int\limits_{-\infty}^{\infty}\frac{dp'}{2\pi}\int\limits_{-\infty}^{\infty}\psi(p')dp'$$

(здесь пренебрегаем p' под косинусом и интегрируем по всему импульсному пространству (одномерному), в итоге справа волновая функция стала 1, слева меняем интегралы местами, потом протаскиваем интеграл до левой волновой функции, и оказывается, что волновая функция тоже уходит)

далее

$$1 = -\int dx\int\frac{dp}{2\pi}\frac{e^{-ipx}}{p^2/(2m)+|E|}\left(\frac{-aU_0}{a+|x|}\right)$$

$$1 = \frac{maU_0}{\pi}\int\frac{dx}{a+|x|}\int\frac{\cos(px)dp}{p^2+2m|E|}$$

(??? преобразование утеряно??)

В итоге

$$\to 1 = \frac{maU_0}{\sqrt{2m|E|}}\int\frac{dxe^{-|x|\sqrt{2m|E|}}}{a+|x|}$$

теперь мы в шаге от нахождения энергии основного состояния, нужно его решить.

введем параметры $t = x\sqrt{2m|E|}$, $\beta = \sqrt{2m|E|}a$.

Считать нужно интеграл с малым β:

$$I = \int \frac{dte^{-|t|}}{\beta + |t|}$$

в нашем случае $\beta \ll |t| \ll 1$, для него решается так:

$$I_2 \approx 2\int\limits_{\beta}^{1} \frac{dt}{\beta + t} \approx 2\ln\frac{1}{\beta}$$

и получаем

$$I \approx 2\ln\frac{1}{\sqrt{2m|E|}a}$$

итог наших действий:

$$1 = \frac{maU_0}{\sqrt{2m|E|}} 2\ln\frac{1}{\sqrt{2m|E|}a} \qquad \leftrightarrow \qquad \frac{a\sqrt{2m|E|}}{ma^2U_0} = -2\ln\sqrt{2m|E|}a$$

короче, хочется сказать, что уровни энергии неявно следуют из этого уравнения.

вообще, так как тут все константы и ищем $|E|$, неплохо бы заменить параметрами и посмотреть просто пересечение графика левой и правой части (как в школе мы делали)

и так как в меня время почти вышло, просто воспользуемся методами, которые советуют математики (это как метод итераций из вычматов):

вводим параметры

$\beta = ma^2U_0 \ll 1$ - константа, $\alpha := a\sqrt{2m|E|}/\beta$ - наша переменная.

уравнение в них $\alpha = -2\ln(\alpha\beta)$

начнем с простейшей зависимости: $\alpha_0 = 1$, тогда на следующем шаге: $\alpha_1 = -2\ln(\beta)$, а потом $\alpha_2 = -2\ln(-2\beta\ln(\beta))$.

если так вообще можно делать, то мы уже с какой-то точностью решили это уравнение.

Добавляя куда нужно $\hbar$, видим:

$$|E| \approx 2U_0 \cdot (ma^2U_0/\hbar)\ln^2(-2ma^2U_0/\hbar\ln(ma^2U_0/\hbar)).$$

Почему самое простейшее решение задачи неверное?

Как известно, задача о трёхмерном Кулоновском потенциале, в частности, при нулевом орбитальном моменте $l = 0$ сводится как раз к одномерной задаче ровно в потенциале $U(x) = -\frac{e^2}{\sqrt{x^2+a^2}}$. Тем самым, казалось бы, ничего не мешает в этом потенциале просто положить $a = 0$ и воспользоваться решением трёхмерной задачи, для которой известно основное состояние $-\psi_{3D}(r) = e^{-r/a_B}$ с энергией $E_0 = -\mathrm{Ry}^{-13} = -me^4/2\hbar^2 = -13.6\mathrm{eV}$

Однако, это рассуждение неверно. Связано это с тем, что переход от трёхмерной задач к одномерной осуществляется подстановкой $\psi_{3D}(r) = \psi_{1D}(r)/r$, и основное состояние трёхмерного Кулона, соответствует одномерной волновой функции $\psi_{1D}(r) = r\exp(-r/a_B)$. У этой волновой функции имеется ровно один узел, $\psi_{1D}(r = 0) = 0$, поэтому по осцилляторной теореме она описывает первое возбуждённое состояние одномерного Кулона! А как же тогда устроено основное?

Оказывается, в одномерии буквально Кулоновский потенциал $U(x) = -\alpha/|x|$ соответствует «падению на центр» и нарушает унитарность - а его основное состояние имеет энергию $E_0 = -\infty$. Для того, чтобы это увидеть, мы и предлагаем ввести «обрезку» потенциала на самых маленьких расстояниях и исследовать поведение энергии основного состояния при $a \to 0$.

(????????? это нужно еще продумать, пока не понял особо глубоко???. в 1ю часть тоже допишу про это)

ФР.? Спектр в экранированном Кулоне

Вычислить, ограничиваясь первым порядком теории возмущений, спектр s-состояний в экранированном кулоновском потенциале $U(r) = -\frac{e^2}{r}e^{-r/\ell}$, при $\ell \gg a_0$. Оценить максимальное n, при котором применима теория возмущений.

Solution.

Обычная теория возмущений дает ответ (????).

Разложим потенциал в ряд по $\frac{1}{\ell}$:

$$U(r) \approx -\frac{e^2}{r}\left(1 - \frac{r}{\ell} + \frac{1}{2}\frac{r^2}{\ell^2}\right) \approx -\frac{e^2}{r} + \frac{e^2}{r}\left(\frac{r}{\ell} - \frac{r^2}{2\ell^2}\right)$$

При $r \ll \ell$ наш потенциал имеет вид $U \approx -e^2/r$. В нулевом приближении искомые уровни нижней части спектра и соответствующие им с.ф. будут такие же, как и в кулоновском поле:

$$E^{(0)}_{n_r l} = -\frac{me^4}{2\hbar^2 n^2}, \quad \Psi^{(0)}_{n_r lm} = \Psi^{\text{кул}}_{n_r lm},$$

При этом отличие рассматриваемых потенциалов от кулоновского играет роль возмущения

$$V(r) = U(r) + e^2/r \approx \frac{e^2}{\ell}$$

Ввиду того что орбитальный момент частицы является интегралом движения и при действии возмущения, с.ф. $\Psi^{(0)}_{n_r lm}$ являются правильными функциями нулевого приближения, поправка первого порядка определяется выражением

$$E^{(1)}_{n_r l} = \int V(r)|\Psi^{(0)}_{n_r lm}|^2 d^3r.$$

Исходя их того, что $\int |\Psi^{(0)}_{n_r lm}|^2 d^3r = 1$, получим:

$$E^{(1)}_{n_r l} = \int \frac{e^2}{\ell}|\Psi^{(0)}_{n_r lm}|^2 d^3r = \frac{e^2}{\ell}.$$

Спектр, то есть энергия состояний, есть:

$$E_n \approx -\frac{me^2}{2\hbar^2 n^2} + \frac{e^2}{\ell}.$$

Определение границ применимости

$$\frac{|V_{kn}|}{\Delta E^{(0)}_{kn}} \ll 1,$$

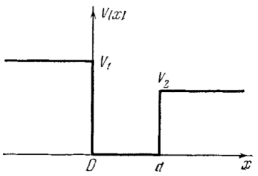
$$\frac{\frac{e^2}{\ell}}{\frac{me^4}{2\hbar^2}\left(-\frac{1}{n^2} + \frac{1}{(n-1)^2}\right)} \approx \frac{2\hbar^2}{m\ell e^2}(n-1)^2 \ll 1,$$

учтено, что $\frac{1}{n^2} \ll \frac{1}{(n-1)^2}$. В итоге получим, что теория возмущений работает для

$$n \ll \sqrt{\frac{m\ell e^2}{2\hbar^2}} + 1$$

ГК-1.4. Несимметричная потенциальная яма

Определить уровни энергии и волновые функции частицы, находящейся в несимметричной потенциальной яме вида



Рассмотреть предельный случай $V_1 = V_2$, и в этом случае предел мелкой ямы.

Solution.

Пишем уравнение Шредингера для каждой области, вводим переменные, подставляем ожидаемые анзацы, сшиваем и получаем выражения для коэффициентов. Для симметричной ямы нужно внимательно посмотреть на имеющиеся уравнения.

$$\begin{aligned}
&\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2} + (E - V_1)\,\psi = 0 \qquad && (x < 0),\\
&\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2} + E\psi = 0 && (0 < x < a),\\
&\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2} + (E - V_2)\,\psi = 0 && (x > a).
\end{aligned}$$

$$\varkappa_1 := \frac{\sqrt{2\mu\,(V_1 - E)}}{\hbar}, \quad \varkappa := \frac{\sqrt{-2\mu E}}{h}, \quad \varkappa_2 := \frac{\sqrt{2\mu\,(V_2 - E)}}{\hbar},$$

$$\begin{aligned}
&\psi = A_1 e^{-\varkappa_2 x} + B_1 e^{\varkappa_1 x} && (x < 0)\\
&\psi = A e^{-\varkappa x} + B e^{\varkappa x} && (0 < x < a),\\
&\psi = A_2 e^{-\varkappa_2 x} + B_2 e^{\varkappa_2 x} && (x > a)
\end{aligned}$$

Рассмотрим дискретный спектр $E < V_2$. Тогда $\varkappa_1$ и $\varkappa_2$-действительные величины. Полагая в средней области $0 < \varkappa < a$, величину $\varkappa = ik$, где k - действительно, поищем решение в виде

$$\psi \sim \sin(kx + \delta) \quad (0 < x < a)$$

В силу конечности волновой функции $A_1 = 0, B_2 = 0$. Из условия непрерывности логарифмической производной $\frac{1}{\psi}\frac{d\psi}{dx}$ получаем

$$\begin{aligned}
\varkappa_1 &= k \operatorname{ctg} \delta\\
-\varkappa_2 &= k \operatorname{ctg}(ka + \delta).
\end{aligned}$$

Перепишем последние два условия, выразив x_1 и x_2 через k

$$\begin{aligned}
&\sqrt{\frac{2\mu V_1}{\hbar^2 k^2} - 1} = \operatorname{ctg} \delta,\\
&-\sqrt{\frac{2\mu V_2}{\hbar^2 k^2} - 1} = \operatorname{ctg}(ka + \delta).
\end{aligned}$$

Запомним сперва, что из этих уравнений следует, что аргументы котангенсов должны находиться в 1-ом или 3-ем и во 2-м и 4-м квадранте соответственно. Возводим в квадрат, переходим к синусу, извлекаем корень, получаем много решений для каждого уравнения, параметризуем их через $n_1, n_2 \in \mathbb{Z}$:

$$\begin{aligned}
\delta &= \arcsin \frac{\hbar k}{\sqrt{2\mu V_1}} + n_1 \pi\\
ka + \delta &= -\arcsin \frac{\hbar k}{\sqrt{2\mu V_2}} + n_2 \pi
\end{aligned}$$

Исключая δ, находим уравнение для определения уровней энергий:

$$ka = n\pi - \arcsin \frac{\hbar k}{\sqrt{2\mu V_1}} - \arcsin \frac{\hbar k}{\sqrt{2\mu V_2}}, \qquad k = \frac{\sqrt{2\mu E}}{\hbar} > 0.$$

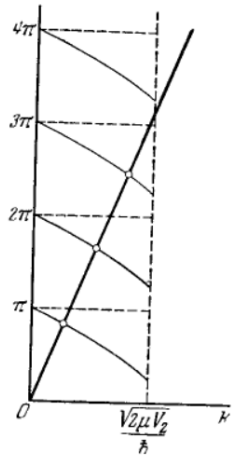
Верность знаков легко проверить, посмотрев на тригонометрическую окружность еще раз. Значения k, удовлетворяющие этому уравнению, можно найти графически. Эти значения определяются точками пересечения прямой

$$y_1(k) = ak$$

и кривыми

$$y_2(k) = n\pi - \arcsin \frac{\hbar k}{\sqrt{2\mu V_1}} - \arcsin \frac{\hbar k}{\sqrt{2\mu V_2}}$$

Имеется конечное число уровней, потому что arcsin вычисляется только для $\sqrt{E} = \frac{\hbar k}{\sqrt{2\mu}} < \sqrt{V_2}$ (ведь $V_2 < V_1$):



Случай симметричной ямы $V_1 = V_2 = V$

Так как $\arcsin \in [-\pi/2, \pi/2]$, то для каждого V и a всегда имеется по крайней мере один k, который удовлетворяет системе уравнений, то есть по крайней мере один уровень.

Для $\frac{\sqrt{2\mu V}}{\hbar}a \ll 1$, находим уровень энергии разложениями:

$$E \approx V - \xi; \qquad k \approx \sqrt{2\mu V}/\hbar$$

$$\sqrt{E/V} \approx 1 - \frac{\xi}{2V},$$

from $\arcsin(1-x) \approx \frac{\pi}{2} - \sqrt{2}x^{1/2}$ (see proof below),

$$\arcsin\sqrt{E/V} \approx \pi/2 - \sqrt{2}\sqrt{\frac{\xi}{2V}}$$

$$\pi - 2\left(\frac{\pi}{2} - \sqrt{\frac{\xi}{V}}\right) = a\sqrt{2\mu V}/\hbar$$

$$\xi = \frac{\mu a^2}{2\hbar^2}V^2.$$

В итоге:

$$E = V - \frac{\mu a^2}{2\hbar^2}V^2.$$

Число уровней N при любых V и найдется из

$$tg\angle = a \equiv N\pi/(\sqrt{2\nu V}/\hbar)$$

т.е. оно определяется соотношением:

$$N > \frac{\sqrt{2\mu V}a}{\pi\hbar} > N - 1$$

(???? я забыл это, переписать нужно решение вообще)

Appendix: derivation of $\arcsin(1-x) \approx \frac{\pi}{2} - \sqrt{2}x^{1/2}$

$$\arcsin x \approx \arcsin(1) + \arcsin'(1)(x-1) = \frac{\pi}{2} + \left(\frac{1}{\sqrt{1-x^2}}\right)\Bigg|_{x=1}(x-1) \overset{\text{Lop. r.}}{=} \frac{\pi}{2} - \frac{\sqrt{1-x^2}}{x} =$$

$$= \frac{\pi}{2} - \frac{\sqrt{1-x^2}}{x}\Bigg|_{x\to 1} = \frac{\pi}{2} - \sqrt{(1-x)(1+x)}\Big|_{x\to 1} = \frac{\pi}{2} - \sqrt{2(1-x)}$$

$$\arcsin x \equiv \arcsin(1-\xi) \qquad \Rightarrow \qquad \xi = 1 - x$$

$$\arcsin(1-\xi) \approx \frac{\pi}{2} - \sqrt{2\xi}$$

Here we have a coefficient $\to \infty$, so we take a limit of a whole term.

Another way:

$$\arcsin(1-\xi) \approx \arcsin(1-0) + \arcsin'(1-\xi)\Big|_{\xi\to 0}\xi = \frac{\pi}{2} - \frac{1}{\sqrt{1-(1-\xi)^2}}\xi \overset{\text{Lop. r.}}{\approx} \frac{\pi}{2} - \sqrt{2\xi}$$

17.2.4 Problems about delta-potentials 1

Б-2.2.6 Уровни энергии в δ-яме

Найти уровень энергии и собственную функцию связанного состояния в δ-яме $U(x) = -\frac{\hbar^2}{m}\varkappa_0\delta(x)$.

Solution..

Это одна из самых известных модельных задач, можно сразу написать ответ.

Положим $E < 0$ и введем

$$\varkappa^2 := \frac{2m|E|}{\hbar^2},$$

$$\psi''(x) - \left(\varkappa^2 - 2\varkappa_0\delta(x)\right)\psi(x) = 0.$$

В точке разрыва потенциала $x = 0$ потребуем непрерывности $\psi(x)$:

$$\psi(+0) = \psi(-0).$$

При этом производная $\psi'(x)$ терпит разрыв, величину которого находим из уравнения Шредингера, интегрируя его в пределах от $-\varepsilon$ до ε при $\varepsilon \to 0$: $\psi'(+0) - \psi'(-0) = -2\varkappa_0\psi(0)$. При этом, как и должно быть, выполняется условие непрерывности плотности потока вероятности: $j(+0) = j(-0)$, где $j(x) = \frac{i\hbar}{2m}\left(\psi(x)\psi'(x)^* - \psi^*(x)\psi'(x)\right)$.

Нормированное решение ищем в виде

$$\psi(x) = \begin{cases} C_1 e^{-\varkappa x}, & x > 0, \\ C_2 e^{\varkappa x}, & x < 0. \end{cases}$$

Из непрерывности ψ при $x = 0$, получаем $C_1 = C_2 = C$. Тогда условие непрерывности производной дает $\varkappa = \varkappa_0$, т. е. при $E < 0$ имеем всего один дискретный уровень с энергией

$$E_0 = -\frac{\hbar^2\varkappa_0^2}{2m}$$

и волновой нормированной функцией

$$\psi_0(x) = \sqrt{\varkappa_0}e^{-\varkappa_0|x|} \equiv \langle x|0\rangle.$$

Б-2.2.7 Средние значения в δ-яме

Для связанного состояния частицы в поле δ-ямы найти $\langle\hat{\mathrm{x}}\rangle, \langle\hat{\mathrm{x}}^2\rangle, \langle\hat{\mathrm{p}}\rangle, \langle\hat{\mathrm{p}}^2\rangle$. Рассмотреть разные способы вычисления $\langle\hat{\mathrm{p}}^2\rangle$. Проверить, выполняется ли соотношение неопределённостей.

Solution..

В импульсном представлении волновая функция дискретного уровня задачи 2.2.6 будет иметь вид

$$\psi_0(p) \equiv \langle p|0\rangle = \int\limits_{-\infty}^{\infty} dx\langle p|x\rangle\langle x|0\rangle = \frac{\sqrt{\varkappa_0}}{(2\pi\hbar)^{1/2}}\int\limits_{-\infty}^{\infty} e^{-\varkappa_0|x| - \frac{ipx}{\hbar}}dx = \sqrt{\frac{2}{\pi}}\frac{(\varkappa_0\hbar)^{3/2}}{(\varkappa_0\hbar)^2 + p^2}.$$

Легко найти $\langle 0|\hat{x}|0\rangle = 0, \langle 0|\hat{\mathrm{p}}|0\rangle = 0$, а также

$$\langle 0|\hat{x}^2|0\rangle = \int\limits_{-\infty}^{\infty} xe^{-2x_0|x|}\hat{x}^2dx = \alpha\int\limits_0^{\infty} e^{-\alpha x}x^2dx = \alpha\frac{d^2}{d\alpha^2}\int\limits_0^{\infty} e^{-\alpha x}dx = \frac{2}{\alpha^2}\Big|_{\alpha=2x_0} = \frac{1}{\varkappa_0^2},$$

и, кроме того,

$$\langle 0|\hat{p}^2|0\rangle = \int\limits_{-\infty}^{\infty} dpp^2 \frac{2}{\pi} \frac{(\varkappa_0\hbar)^3}{\left((\hbar\varkappa_0)^2+p^2\right)^2} = \frac{2}{\pi}(\varkappa_0\hbar)^3 \left(-\frac{d}{d\alpha^2}\right) \int\limits_{-\infty}^{\infty} \frac{p^2dp}{\alpha^2+p^2} =$$
$$= \frac{2}{\pi}(\varkappa_0\hbar)^3 \left(-\frac{d}{d\alpha^2}\right) \frac{2\pi i(i\alpha)^2}{2i\alpha}\bigg|_{\alpha=\varkappa\hbar} = (\varkappa_0\hbar)^2$$

Соотношение неопределённостей для данного состояния имеет вид

$$\langle(\Delta\hat{x})^2\rangle\langle(\Delta\hat{\mathrm{p}})^2\rangle = \frac{1}{2\varkappa_0^2}\varkappa_0^2\hbar^2 = \frac{\hbar^2}{2} > \frac{\hbar^2}{4}$$

- абсолютный минимум для когерентного состояния гармонического осциллятора.

Б-2.2.8 δ-яма в импульсном представлении (!?!?!)

Найти энергию и волновые функции в поле δ-ямы $U(x) = -\frac{\hbar^2}{m}\varkappa_0\delta(x)$ в импульсном представлении.

Solution..

(тут про это хорошие ходы, вот это решить еще раз нужно!)

Фурье-образ потенциала равен константе, и уравнение Шредингера в импульсном представлении принимает простой вид:

$$\frac{p^2}{2m}\varphi(p) + \frac{\hbar\varkappa_0}{2\pi m}\int\limits_{-\infty}^{\infty} dp'\varphi(p') = E\varphi(p)$$

$$E = -\hbar^2\varkappa^2/(2m) < 0 \qquad\qquad C := \int\limits_{-\infty}^{\infty} dp'\varphi(p')\,.$$

$$\varphi(p) = \frac{\hbar\varkappa_0}{\pi}\frac{C}{p^2+\hbar^2\varkappa^2}.$$

Еще раз интегрируем:

$$C = \frac{\hbar\varkappa_0}{\pi}\int\limits_{-\infty}^{+\infty}\frac{C}{(p^2+\hbar^2\varkappa^2)}dp = C\frac{\varkappa_0}{\varkappa},$$

$$E = -\frac{\hbar^2\varkappa_0^2}{2m}.$$

$$\int\limits_{-\infty}^{+\infty}|\varphi(p)|^2dp = 1, \qquad \Rightarrow \qquad |C|^{-2} = \left(\frac{\hbar\varkappa_0}{\pi}\right)^2\int\limits_{-\infty}^{+\infty}\frac{dp}{\left(p^2+\hbar^2\varkappa_0^2\right)^2}.$$

Вычисляем вычетами: следует взять вычет в полюсе второго порядка, например в верхней полуплоскости в точке $z = i\hbar\varkappa_0$, после чего получаем $C = \sqrt{2\pi\hbar\varkappa_0}$. В итоге

$$\psi_\rho = \sqrt{\frac{2}{\pi\hbar\varkappa_0}}\frac{1}{p^2/\hbar^2\varkappa_0^2+1}$$

в полном соответствии с

$$\psi_0(p) \equiv \langle p|0\rangle = \int\limits_{-\infty}^{\infty} dx\langle p|x\rangle\langle x|0\rangle = \frac{\sqrt{\varkappa_0}}{(2\pi\hbar)^{1/2}}\int\limits_{-\infty}^{\infty} e^{-\varkappa_0|x|-\frac{ipx}{\hbar}}dx = \sqrt{\frac{2}{\pi}}\frac{(\varkappa_0\hbar)^{3/2}}{(\varkappa_0\hbar)^2+p^2}$$

Б-2.2.10 Последовательность дельта-потенциалов

Найти разрешенные зоны энергии для частицы, движущейся в одномерном периодическом поле вида

а) $U(x) = \sum\limits_{n=-\infty}^{\infty}\frac{\hbar^2\beta_0}{m}\delta(x-na)$ (модель Кронига-Пенни);

б) $U(x) = -\sum\limits_{n=-\infty}^{\infty}\frac{\hbar^2x_0}{m}\delta(x-na)$.

Рассмотреть предельные случаи $\beta_0 a \gg 1$ (или $\varkappa_0 a \gg 1$, сильная связь) и $\beta_0 a \ll 1$ (или $\varkappa_0 a \ll 1$, слабая связь).

а) Модель Кронига-Пенни

Вследствие инвариантности потенциала относительно трансляций на величину периода одномерной кристаллической решетки a, т. е. $U(x+a)=U(x)$, гамильтониан нашей задачи будет коммутировать с оператором трансляции $\hat{\mathrm{T}}_a$:

$$\left[\hat{\mathrm{H}},\hat{\mathrm{T}}_a\right]=0.$$

Поэтому мы можем искать решение в виде общих собственных функций операторов $\hat{\mathrm{H}}$ и $\hat{\mathrm{T}}_a$:

$$\begin{cases}\hat{\mathrm{H}}\psi(x)=E\psi(x),\\ \hat{\mathrm{T}}_a\psi(x)=\lambda(a)\psi(x),\end{cases}$$

где $\lambda(a)$ (собственное значение оператора трансляции) имеет вид $\lambda(a)=e^{\pm iKa}$, а $\operatorname{Im}K=0$ (квазиимпульс). Собственные функции оператора трансляции согласно теореме Блоха должны удовлетворять условию, которое следует из (1):

$$\psi(x+a)=e^{iKa}\psi(x)$$

Запишем общий вид решения уравнения Шредингера (1) в двух смежных областях:

$0<x<a$ (область 1): $\psi(x)=c_1e^{ikx}+d_1e^{-ikx}$,

$a<x<2a$(область 2) : $\psi(x)=c_2e^{ik(x-a)}+d_2e^{-ik(x-a)}$,

причем $E=\frac{\hbar^2k^2}{2m}>0$.

Условия сшивания в точке $x=a$

$$\psi(a+0)=\psi(a-0),$$
$$\psi'(a+0)-\psi'(a-0)=2\beta_0\psi(0)$$

после элементарных вычислений дают связь между коэффициентами $c_1,\ d_1, c_2, d_2$, которую можно записать в матричном виде:

$$\begin{pmatrix}c_2\\ d_2\end{pmatrix}=A\begin{pmatrix}c_1\\ d_1\end{pmatrix},\qquad A:=\begin{pmatrix}e^{ika}\left(1+\frac{\beta_0}{ik}\right) & e^{-ika}\frac{\beta_0}{ik}\\ -e^{ika}\frac{\beta_0}{ik} & e^{-ika}\left(1-\frac{\beta_0}{ik}\right)\end{pmatrix}.$$

Нетрудно заметить, что $\det A=1$. Далее мы применим формулу (2) и получим

$$\psi(x+a)=c_2e^{ik(x+a-a)}+d_2e^{-ik(x+a-a)}=c_2e^{ikx}+d_2e^{-ikx}=e^{iKa}\psi(x).$$

Таким образом, имеем

$$\begin{pmatrix}c_2\\ d_2\end{pmatrix}=e^{iKa}\begin{pmatrix}c_1\\ d_1\end{pmatrix},$$

и, сравнивая (3) и (4), видим, что задача свелась к проблеме диагонализации матрицы A (матрица сдвига), а $e^{iKa}=\lambda(a)$ - играет роль собственного значения этой матрицы. В результате получаем уравнение на собственные значения

$$\lambda^2(a)-2\rho\lambda(a)+1=0,$$

где $2\rho=\mathrm{Sp}A$ - след матрицы A. Решение уравнения дает

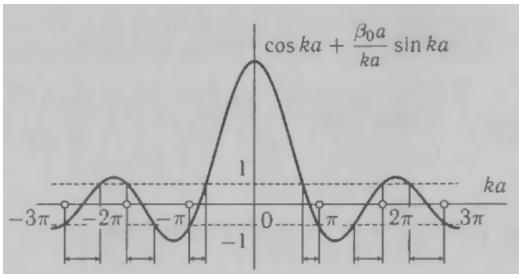
$$\lambda_{1,2}(a)=e^{\pm iKa}=\rho\pm i\sqrt{1-\rho^2},$$

откуда следует, что $\cos Ka=\rho$ или, конкретнее:

$$\cos Ka=\cos ka+\frac{\beta_0}{k}\sin ka.$$

Это и есть так называемое дисперсионное соотношение.

Анализ соотношения (5) показывает, что энергетический спектр частицы в таком поле имеет зонную структуру. В самом деле, задавшись некоторым значением энергии E, мы находим $k=\sqrt{2mE}/\hbar$ и затем из уравнения (5) можем найти значение a (рис. 2.4).



Случай 1. Энергия E такова, что $|\rho| = |\cos Ka| \leqslant 1$. При этом K является вещественным числом, что и требуется для функции Блоха, а сама функция - распространяющаяся модулированная волна. Эти области значений E называются разрешенными зонами энергии.

Случай 2. Энергия E такова, что $|\rho| = |\cos Ka| > 1$. При этом величина K - комплексная, и частицы с такими K не могут распространяться внутри большого кристалла. Эти области значений энергии запрещенные зоны.

Разрешенные зоны чередуются с запрещенными, не перекрываясь между собой. Ширина разрешенных зон увеличивается с ростом $|ka|$. Условие $\beta_0 a \ll 1$ (слабая связь) описывает случай, близкий к свободному. Это значит, что $K \simeq k + 2\pi n/a$, и поэтому зависимость $E(K)$ параболическая. В противоположном предельном случае $\beta_0 a \gg 1$ (сильная связь) интервалы разрешенных значений энергии фактически превращаются в отдельные дискретные уровни $ka \approx \pi n$.

б) Модель Кронига-Пенни с обратным знаком

(?? то же самое, только все со знаком минус будет? потом подумаю.)

Б-2.2.12 Переход из одной дельта-ямы в другую (!?)

Пусть имеется два дельта потенциала с $\varkappa_0 a \gg 1$. Пусть частица в начальный момент времени $t = 0$ находится в левой яме. Найти вероятность обнаружения частицы в правой яме в момент времени t.

Предполагаются следующие приближения:

а) δ-ямы находятся достаточно далеко друг от друга, т. е. в системе ям имеется два дискретных уровня энергии, отвечающих связанным состояниям. Однако ямы не бесконечно далеки, следовательно, $E^{(+)} \neq E^{(-)}$.

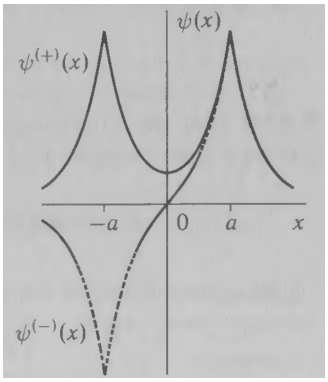
б) Система, рассматриваемая нами, - приближенно двухуровневая, т. е. отброшен весь непрерывный спектр - считается, что частица не выходит из ям.

Solution.

Как это следует из рис. 2.5, в любом из стационарных состояний $\psi^{(+)}(x)$ или $\psi^{(-)}(x)$ выполняется

$$|\psi^{(\pm)}(-x)|^2 = |\psi^{(\pm)}(x)|^2,$$

поэтому вероятность обнаружения частицы вблизи левой и правой ямы одинакова - частица не локализована вблизи ни одной из ям.



С целью построить состояние, в котором частица (хотя бы в начальный момент времени) была бы локализована в окрестности одной из ям, воспользуемся линейной комбинацией функций

$$\Psi(x,t) = C_1 e^{-\frac{iE^{(+)}t}{\hbar}} \psi^{(+)}(x) + C_2 e^{-\frac{iE^{(-)}t}{\hbar}} \psi^{(-)}(x).$$

Очевидно, что в начальный момент времени

$$\Psi(x,0) = C_1 \psi^{(+)}(x) + C_2 \psi^{(-)}(x)$$

Если положить $C_1 = C_2$, то мы получим состояние (рис. 2.5), в котором частица локализована вблизи правой δ-ямы. Обозначим это состояние $\Psi(x,0) = \psi_a(x)$. По аналогии можно построить состояние $\psi_{-a}(x)$ с локализацией частицы вблизи левой δ-ямы. Окончательно

$$\begin{cases} \psi_a(x) = \dfrac{1}{\sqrt{2}}\left(\psi^{(+)}(x) + \psi^{(-)}(x)\right), \\ \psi_{-a}(x) = \dfrac{1}{\sqrt{2}}\left(\psi^{(+)}(x) - \psi^{(-)}(x)\right), \end{cases} \quad \Leftrightarrow \quad \begin{cases} \psi^{(+)}(x) = \dfrac{1}{\sqrt{2}}\left(\psi_a(x) + \psi_{-a}(x)\right), \\ \psi^{(-)}(x) = \dfrac{1}{\sqrt{2}}\left(\psi_a(x) - \psi_{-a}(x)\right). \end{cases}$$

Итак, волновая функция состояния (1), в котором частица в начальный момент времени локализована вблизи правой δ-ямы, имеет вид

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left\{e^{-\frac{iE^{(+)}t}{\hbar}}\psi^{(+)}(x) + e^{-\frac{iE^{(-)}t}{\hbar}}\psi^{(-)}(x)\right\} = \\ = \frac{1}{2}\left\{\psi_a(x)\left[e^{-\frac{iE^{(+)}t}{\hbar}} + e^{-\frac{iE^{(-)}t}{\hbar}}\right] + \psi_{-a}(x)\left[e^{-\frac{iE^{(+)}t}{\hbar}} - e^{-\frac{iE^{(-)}t}{\hbar}}\right]\right\}.$$

Тогда вероятность обнаружить частицу локализованной вблизи левой ямы, если в начальный момент она была в правой, равна

$$W_{-a} = \frac{1}{4}|e^{-\frac{iE^{(+)}t}{\hbar}} - e^{-\frac{iE^{(-)}t}{\hbar}}|^2 = \frac{1}{2}\left[1 - \cos\left(\frac{E^{(+)} - E^{(-)}}{\hbar}t\right)\right] = \sin^2\left[\frac{E^{(+)} - E^{(-)}}{2\hbar}t\right].$$

ПТФ-3.з3.1/2. Туннельное расщепление

Рассмотрите две мелкие ямы, моделируемые следующим потенциалом:

$$U(x) = -\frac{\hbar^2\kappa}{m}(\delta(x + L/2) + \delta(x - L/2))$$

• Нарисуйте (схематично, но со всеми ключевыми особенностями) зависимость уровней энергии связанных состояний от расстояния между ямами L.
• Пусть расстояние между ямами много больше характерного масштаба волновых функций для каждой из отдельных ям (туннельный режим), $L \gg \kappa^{-1}$. Определите расщепление между связанными состояниями.
• Эта задача может быть рассмотрена как модель ковалентной связи. Считая теперь L классической динамической переменной, определите силу (в туннельном режиме) и характер взаимодействия между ямами, если частица находится в основном состоянии.

Поиск зависимости энергии от расстояния

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E - U(x))\psi(x) = E\psi(x)$$

$$E < 0$$

$$k^2 := -\frac{2mE}{\hbar^2}.$$

For even states:

$$\psi_{\text{even}}(x) = \begin{cases}\psi_I(x) = Ae^{kx}, & x < -\frac{L}{2} \\ \psi_{II}(x) = B\cosh kx, & -\frac{L}{2} < x < \frac{L}{2} \\ \psi_{III}(x) = Ae^{-kx}, & x > \frac{L}{2}\end{cases}$$

$$\psi_{II}\left(\frac{L}{2}\right) = \psi_{III}\left(\frac{L}{2}\right), \quad \psi'_{III}\left(\frac{L}{2}\right) - \psi'_{II}\left(\frac{L}{2}\right) = -2\varkappa\psi_{III}\left(\frac{L}{2}\right)$$

$$Ae^{-\frac{kL}{2}} = B\cosh\frac{kL}{2}, \quad A(2\kappa - k)e^{-\frac{kL}{2}} = kB\sinh\frac{kL}{2}$$

(я потом допишу вывод там нужно приблизить sh и ch и чуть преобразовать, что ниже и получится)

$$1 + e^{-y} = \frac{y}{\kappa L}, \qquad y := kL$$

Это трансцендентное уравнение.

$$E_{\text{odd}} = -\frac{\hbar^2k^2}{2m} = -\frac{\hbar^2y^2}{2mL^2} \qquad y: \quad 1 + e^{-y} = \frac{y}{\kappa L}$$

Now, for odd states:

$$\psi_{\text{odd}}(x) = \begin{cases}\psi_I(x) = Ae^{kx}, & x < -\frac{L}{2} \\ \psi_{II}(x) = B\sinh kx, & -\frac{L}{2} < x < \frac{L}{2} \\ \psi_{III}(x) = -Ae^{-kx}, & x > \frac{L}{2}\end{cases}$$

Запишем граничные условия (из чётности достаточно их записать в одной точке $x = \frac{L}{2}$):

$$\psi_{II}\left(\frac{L}{2}\right) = \psi_{III}\left(\frac{L}{2}\right), \quad \psi'_{III}\left(\frac{L}{2}\right) - \psi'_{II}\left(\frac{L}{2}\right) = -2\kappa\psi_{III}\left(\frac{L}{2}\right)$$

$$Ae^{-\frac{kL}{2}} = B\sinh\frac{kL}{2}, \quad A(2\kappa - k)e^{-\frac{kL}{2}} = kB\cosh\frac{kL}{2}$$

$$1 - e^{-y} = \frac{y}{\kappa L}, \qquad y := kL$$

Получилось трансцендентное уравнение.

$$E_{\text{odd}} = -\frac{\hbar^2 k^2}{2m} = -\frac{\hbar^2 y^2}{2mL^2} \qquad 1 - e^{-y} = \frac{y}{\kappa L}$$

Графики зависимостей E_1 и E_2 от κL представлены на рис. 1.

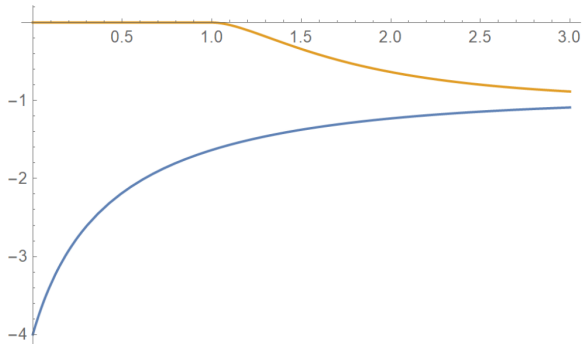


Figure 17.1: Графики зависимостей $E_{\text{even}}(\kappa L)$ (синий график) и $E_{\text{odd}}(\kappa L)$ (жёлтый график)

(надо бы проверить графики, запрограммировать, пока верю. вообще, есть еще другие графики, не уверен, верные ли они. так или иначе, это запросто проверить чуть что можно.)
(??? качественно, почему так и что это значит? у нас только четные в.ф. будут, ибо мин энергия в них?)

Поиск расщепления

• В туннельном режиме (при $\kappa L \gg 1$) решаем методом последовательных приближений (here even→ 1, odd→ 2):

$$y_1^{(0)} = y_2^{(0)} = \kappa L$$

$$y_1^{(1)} = \kappa L(1 + e^{-\kappa L}), \qquad y_2^{(1)} = \kappa L(1 - e^{-\kappa L})$$

$$E_1 = -\frac{\hbar^2\kappa^2}{2m}(1 + 2e^{-\kappa L}) + \mathcal{O}(e^{-2\kappa L}), \qquad E_2 = -\frac{\hbar^2\kappa^2}{2m}(1 - 2e^{-\kappa L}) + \mathcal{O}(e^{-2\kappa L})$$

$$\Delta E = E_2 - E_1 = \frac{2\hbar^2\kappa^2 e^{-\kappa L}}{m} + \mathcal{O}(e^{-2\kappa L})$$

$$\Delta E = \frac{2\hbar^2\kappa_0^2 e^{-\kappa L}}{m} + \mathcal{O}(e^{-2\kappa L})$$

Случай $\kappa L \gg 1$

(тут мое давнее решение, перепишу потом, оно сейчас криво написано, но идея понятна)
Смотря на решения, видим, что они будут почти κ.
Более точно сделаем итерациями:

$$\frac{\kappa_0 l}{L\kappa} = 1 + \exp(-\kappa_0 L)$$
$$(\kappa_0 L)_0 = L\kappa;$$
$$(\kappa_0 L)_1 = (\kappa_0 L)_0 + \epsilon = L\kappa + \epsilon, \quad \epsilon \ll (\kappa_0 L)_0;$$
$$1 + \frac{\epsilon}{L\kappa} = 1 + \exp(-L\kappa)\exp(\epsilon)$$
$$\epsilon = L\kappa\exp(-L\kappa).$$

Короче говоря, мы получили

$$\kappa_0^{e,o} = \kappa(1 \pm \exp(-L\kappa)).$$

Вспоминая, что $\kappa_0 \equiv \sqrt{\frac{2mE_0}{\hbar^2}}$, находим уровни энергии

$$E_0 = -\frac{\hbar^2}{2m}(\kappa(1+e^{-L\kappa}))^2 \approx \frac{\hbar^2}{2m}\kappa^2(1+2e^{-L\kappa})$$

Сила $F = -\frac{\partial}{\partial l}E_0(L) = -\frac{\hbar^2\kappa^2}{m}\kappa e^{-L\kappa} \approx -\frac{\hbar^2\kappa^3}{m}e^{-L\kappa}$.

Случай $\kappa L \ll 1$

Введем $p = \kappa_0/\kappa$ и

$$p = 1 + \exp(-p\kappa L) \approx 1 + 1 - p\kappa Lp = \frac{2}{1+\kappa l} \approx 2(1-\kappa L).$$

в этом случае будет

$$\kappa_0 = 2\kappa(1-\kappa L).$$

(??? перепроверю. это нужно? мб в условие добавить это?)

Поиск силы взаимодействия

Основное состояние – состояние с минимально допустимой энергией. В туннельном режиме (при $\kappa L \gg 1$) минимальная энергия

$$E_1(L) = -\frac{\hbar^2\kappa^2}{2m}(1+2e^{-\kappa L}) + \mathcal{O}(e^{-2\kappa L})$$

$$F = -\frac{\partial E_1}{\partial L} = -\frac{\hbar^2\kappa^3 e^{-\kappa L}}{m} + \mathcal{O}(e^{-2\kappa L})$$

Поскольку $F < 0$, то ямы притягиваются.

ПТФ-3.з3.2/2. Модель сильной связи

Рассмотрите две мелкие ямы, моделируемые следующим потенциалом:

$$U(x) = -\frac{\hbar^2\kappa}{m}(\delta(x+L/2) + \delta(x-L/2))$$

В туннельном данный потенциал может моделировать сильную связь для пары нижних уровней энергии. Все вычисления в этой задаче необходимо проводить в ведущем приближении по параметру $L \gg \kappa^{-1}$.

1. Спроецируйте гамильтониан на линейное подпространство, натянутое на собственные функции каждой из ям по отдельности: $\{|\psi_1\rangle, |\psi_2\rangle\} = \{\psi_0(x+L/2), \psi_0(x-L/2)\}$. Выпишите соответствующую ему матрицу 2×2 в этом базисе.

2. Обратите внимание, что базисные вектора не являются ортогональными. Вычислите матрицу Грама для этого базиса (матрица скалярных произведений $G_{ij} = \langle\psi_i|\psi_j\rangle$).

3. Характеристическое уравнение, определяющее собственные числа для неортонормированного базиса, имеет вид $\det(\hat{H} - E\cdot\hat{G}) = 0$. Найдите собственные уровни энергии в заданном приближении.

Подсказка: обратите внимание: гамильтониан задачи можно записать в виде $\hat{H} = \hat{T} + \hat{U}_1 + \hat{U}_2$, и состояния $|\psi_{1,2}\rangle$ являются собственными для $\hat{H}_{1,2} = \hat{T} + \hat{U}_{1,2}$ соответственно. Это обстоятельство может значительно упростить вычисления. Кроме того, предлагается заметить, что некоторые члены имеет экспоненциальную зависимость $\propto \exp(-\kappa L)$, а часть – зависимость $\propto \exp(-2\kappa L)$, в связи с чем их в ведущем порядке можно положить нулём.

Подготовка к решению

Получим еще раз известные результаты, но в обозначениях данной задачи.

$$\hat{H} = \hat{T} + \hat{U}_1 + \hat{U}_2, \quad \hat{U}_1 = -\frac{\hbar^2\kappa}{m}\delta(x + L/2), \quad \hat{U}_2 = -\frac{\hbar^2\kappa}{m}\delta(x - L/2)$$

$$\hat{H}_1 = \frac{\hat{p}^2}{2m} - \frac{\hbar^2\kappa}{m}\delta(x + L/2), \quad \hat{H}_2 = \frac{\hat{p}^2}{2m} - \frac{\hbar^2\kappa}{m}\delta(x - L/2)$$

$$\hat{H}_i|\psi_i\rangle = E|\psi_i\rangle$$

$$k^2 := -\frac{2mE}{\hbar^2}.$$

$$\hat{H}_1 \qquad \Rightarrow \qquad \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2\kappa}{m}\delta(x + L/2)\right)\psi = E\psi$$

$$\psi(x) = \begin{cases}\psi_I(x) = Ae^{kx}, & x < -\frac{L}{2} \\ \psi_{II}(x) = Be^{-kx}, & x > -\frac{L}{2}\end{cases}$$

$$\psi_I\left(-\frac{L}{2}\right) = \psi_{II}\left(-\frac{L}{2}\right), \quad \psi'_{II}\left(-\frac{L}{2}\right) - \psi'_I\left(-\frac{L}{2}\right) = -2\kappa\psi_{II}\left(-\frac{L}{2}\right)$$

$$Ae^{-\frac{kL}{2}} = Be^{\frac{kL}{2}}, \quad -kBe^{\frac{kL}{2}} - kAe^{-\frac{kL}{2}} = -2\kappa Be^{\frac{kL}{2}}$$

$$B = Ae^{-kL}, \quad k = \kappa$$

$$\psi_1(x) = C_1 e^{-\kappa|x+L/2|}$$

$$\langle\psi_1|\psi_1\rangle = \int\limits_{-\infty}^{\infty} C_1^2 e^{-\kappa|2x+L|}dx = 2C_1^2\int\limits_{0}^{\infty} e^{-2kx}dx = \frac{C_1^2}{k} = 1 \to C_1 = \sqrt{k} = \sqrt{\kappa}$$

$$\psi_1(x) = \sqrt{\kappa}e^{-\kappa|x+L/2|}$$

$$E = -\frac{\hbar^2\kappa^2}{2m}$$

$$\hat{H}_2 \qquad \Rightarrow \qquad \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2\kappa}{m}\delta(x - L/2)\right)\psi = E\psi$$

$$\psi(x) = \begin{cases}\psi_I(x) = Ae^{kx}, & x < \frac{L}{2} \\ \psi_{II}(x) = Be^{-kx}, & x > \frac{L}{2}\end{cases}$$

$$\psi_I\left(\frac{L}{2}\right) = \psi_{II}\left(\frac{L}{2}\right), \quad \psi'_{II}\left(\frac{L}{2}\right) - \psi'_I\left(\frac{L}{2}\right) = -2\kappa\psi_{II}\left(\frac{L}{2}\right)$$

$$Ae^{\frac{kL}{2}} = Be^{-\frac{kL}{2}}, \quad -kBe^{-\frac{kL}{2}} - kAe^{\frac{kL}{2}} = -2\kappa Be^{-\frac{kL}{2}}$$

$$B = Ae^{kL}, \quad k = \kappa$$

$$\psi_2(x) = C_2 e^{-\kappa|x-L/2|}$$

$$\langle\psi_2|\psi_2\rangle = \int\limits_{-\infty}^{\infty} C_2^2 e^{-\kappa|2x-L|}dx = 2C_2^2\int\limits_{0}^{\infty} e^{-2kx}dx = \frac{C_2^2}{k} = 1 \to C_2 = \sqrt{k} = \sqrt{\kappa}$$

$$\psi_2(x) = \sqrt{\kappa}e^{-\kappa|x-L/2|}$$

$$E = -\frac{\hbar^2\kappa^2}{2m}$$

Вычисление проекций

$$\langle\psi_1|\hat{H}|\psi_1\rangle = \langle\psi_1|\hat{H}_1 - \frac{\hbar^2\kappa}{m}\delta(x-L/2)|\psi_1\rangle = E - \frac{\hbar^2\kappa}{m}\langle\psi_1|\delta(x-L/2)|\psi_1\rangle = \\ = -\frac{\hbar^2\kappa^2}{2m}(1+2e^{-2\kappa L}) = -\frac{\hbar^2\kappa^2}{2m}(1+\mathcal{O}(e^{-2\kappa L}))$$

$$\langle\psi_2|\hat{H}|\psi_2\rangle = \langle\psi_2|\hat{H}_2 - \frac{\hbar^2\kappa}{m}\delta(x+L/2)|\psi_2\rangle = E - \frac{\hbar^2\kappa}{m}\langle\psi_2|\delta(x+L/2)|\psi_2\rangle = \\ = -\frac{\hbar^2\kappa^2}{2m}(1+2e^{-2\kappa L}) = -\frac{\hbar^2\kappa^2}{2m}(1+\mathcal{O}(e^{-2\kappa L}))$$

$$\langle\psi_1|\hat{H}|\psi_2\rangle = \langle\psi_1|\hat{H}_2 - \frac{\hbar^2\kappa}{m}\delta(x+L/2)|\psi_2\rangle = \\ = E\langle\psi_1|\psi_2\rangle - \frac{\hbar^2\kappa}{m}\langle\psi_1|\delta(x-L/2)|\psi_2\rangle = \\ = -\frac{\hbar^2\kappa^3}{2m}\int\limits_{-\infty}^{\infty} e^{-\kappa(|x+L/2|+|x-L/2|)}dx - \frac{\hbar^2\kappa^2}{m}e^{-\kappa L} = \\ = -\frac{\hbar^2\kappa^3}{2m}\left(\int\limits_{-\infty}^{-L/2} e^{2\kappa x}dx + \int\limits_{-L/2}^{L/2} e^{-\kappa L}dx + \int\limits_{L/2}^{\infty} e^{-2\kappa x}dx\right) - \frac{\hbar^2\kappa^2}{m}e^{-\kappa L} = \\ = -\frac{3\hbar^2\kappa^2}{2m}e^{-\kappa L} - \frac{\hbar^2\kappa^3 L}{2m}e^{-kL} = \\ = -\frac{\hbar^2\kappa^2}{2m}e^{-\kappa L}(3+\kappa L)$$

$$\langle\psi_2|\hat{H}|\psi_1\rangle = \langle\hat{H}^\dagger\psi_2|\psi_1\rangle = \langle\hat{H}\psi_2|\psi_1\rangle = \langle\psi_1|\hat{H}\psi_2\rangle^\dagger = \langle\psi_1|\hat{H}\psi_2\rangle = -\frac{\hbar^2\kappa^2}{2m}e^{-\kappa L}(3+\kappa L)$$

$$\hat{H} = \begin{pmatrix} -\frac{\hbar^2\kappa^2}{2m}(1+\mathcal{O}(e^{-2\kappa L})) & -\frac{\hbar^2\kappa^2}{2m}e^{-\kappa L}(3+\kappa L) \\ -\frac{\hbar^2\kappa^2}{2m}e^{-\kappa L}(3+\kappa L) & -\frac{\hbar^2\kappa^2}{2m}(1+\mathcal{O}(e^{-2\kappa L})) \end{pmatrix}$$

Let's find the Gram matrix:

$$G_{ii} = \langle\psi_i,\psi_i\rangle = 1$$

$$G_{12} = G_{21} = \langle\psi_1,\psi_2\rangle = \int\limits_{-\infty}^{\infty}\psi_1(x)\psi_2(x)dx = e^{-\kappa L}(1+\kappa L)$$

$$G = \begin{pmatrix} 1 & e^{-\kappa L}(\kappa L+1) \\ e^{-\kappa L}(\kappa L+1) & 1 \end{pmatrix}$$

Поиск собственных уровней

$$\hat{H} - E\hat{G} = \begin{pmatrix} -\frac{\hbar^2\kappa^2}{2m} - E & -e^{-\kappa L}(\frac{\hbar^2\kappa^2}{2m}(3+\kappa L) + E(\kappa L+1)) \\ -e^{-\kappa L}(\frac{\hbar^2\kappa^2}{2m}(3+\kappa L) + E(\kappa L+1)) & -\frac{\hbar^2\kappa^2}{2m} - E \end{pmatrix}$$

$$\det(\hat{H} - E\hat{G}) = 0$$

$$\left(\frac{\hbar^2\kappa^2}{2m} + E\right)^2 - e^{-2\kappa L}\left(\frac{\hbar^2\kappa^2}{2m}(3+\kappa L) + E(\kappa L+1)\right)^2 = 0$$

$$\frac{\hbar^2\kappa^2}{2m} + E = \pm e^{-\kappa L}\left(\frac{\hbar^2\kappa^2}{2m}(3+\kappa L) + E(\kappa L+1)\right)$$

$$E(1 \mp e^{-\kappa L}(\kappa L + 1)) = \frac{\hbar^2\kappa^2}{2m}(\pm e^{-\kappa L}(3 + \kappa L) - 1)$$
$$E = -\frac{\hbar^2\kappa^2}{2m}(1 \pm 2e^{-\kappa L}) + \mathcal{O}(e^{-2\kappa L})$$

Как видно, формулы в туннельном режиме и итоговая тут формула совпадают.

Вычисление проекций более явным способом

Приведу более компактное решение, которое показывает лучше, как делаются вычисления. Смотрим на ямы по отдельности и для них решения:

$$\psi^-(x) = \sqrt{\kappa}\ e^{-\kappa|x-L/2|};$$
$$\psi^+(x) = \sqrt{\kappa}\ e^{-\kappa|x+L/2|}$$

Считаем матрицу Грамма:

$$\langle\psi^+|\psi^+\rangle = \langle\psi^-|\psi^-\rangle = 1;$$
$$\langle\psi^-|\psi^+\rangle = \langle\psi^+|\psi^-\rangle = \kappa\int e^{-\kappa(|x-L/2|-|x+L/2|)}dx = \kappa\left(2\int\limits_{L/2}^{\infty} e^{-2\kappa x}dx + 2\int\limits_{0}^{L/2} e^{-\kappa l}dx\right) = e^{-\kappa l}(\kappa L + 1).$$

$$\hat{G} = \begin{pmatrix} 1 & (\kappa L+1)e^{-\kappa l} \\ (\kappa L+1)e^{-\kappa l} & 1 \end{pmatrix}$$

Считаем гамильтониан в проекциях:

$$\begin{aligned}\langle\psi^-|\hat{H}|\psi^-\rangle &= \frac{-\kappa\hbar^2}{2m}\int e^{-\kappa|x-L/2|}\left(\frac{\partial^2}{\partial x^2} + 2\kappa(\delta(x-L/2)+\delta(x+L/2))\right)e^{-\kappa|x-L/2|}dx = \\ &= -\kappa\frac{\hbar^2}{2m}\left(\left(\int e^{-2\kappa|x-L/2|}(\kappa^2 - \kappa\cdot 2\delta(x-L/2))dx\right) + 2\kappa + 2\kappa e^{-2\kappa l}\right) = \\ &= -\kappa\frac{\hbar^2}{2m}(\kappa - 2\kappa + 2\kappa + 2\kappa e^{-2\kappa l}) = \\ &= \frac{-\kappa^2\hbar^2}{2m}(1 + 2e^{-2\kappa l})\end{aligned}$$

Тут на второй члены в самой внутренней скобке появились за счет второй производной, вне интеграла члены появились от двух дельта функций. Учтено, что производная сигнума - это удвоенная дельта-функция.

$$\begin{aligned}\langle\psi^-|\hat{H}|\psi^+\rangle &= -\kappa\frac{\hbar^2}{2m}\left(\left(\int e^{-\kappa|x-L/2|-\kappa|x+L/2|}(\kappa^2 - \kappa\cdot 2\delta(x-L/2))dx\right) + 4\kappa e^{-\kappa l}\right) = \\ &= -\kappa^2\frac{\hbar^2}{2m}\left(e^{-\kappa l}(\kappa L+1) - 2e^{-\kappa l} + 4e^{-\kappa l}\right) = -\kappa^2\frac{\hbar^2}{2m}\left(e^{-\kappa l}(\kappa L+3)\right)\end{aligned}$$

$$\langle\psi^+|\hat{H}|\psi^-\rangle = -\kappa^2\frac{\hbar^2}{2m}\left(e^{-\kappa l}(\kappa L+3)\right)$$
$$\langle\psi^+|\hat{H}|\psi^+\rangle = \frac{-\kappa^2\hbar^2}{2m}(1 + 2e^{2-\kappa l})$$

В итоге:

$$\hat{H}_P = \frac{-\kappa^2\hbar^2}{2m}\begin{pmatrix} 1+2e^{-2\kappa l} & e^{-\kappa l}(\kappa L+1) \\ e^{-\kappa l}(\kappa L+1) & 1+2e^{-2\kappa l}\end{pmatrix}$$

ищем собственные значения из $\det(\hat{H} - \lambda\hat{G}) = 0$

$$\det\begin{pmatrix} 1+2e^{-2\kappa l} + \lambda\frac{2m}{\kappa^2\hbar^2} & e^{-\kappa l}(3+\kappa L) + \lambda\frac{2m}{\kappa^2\hbar^2}(\kappa L+3)e^{-\kappa l} \\ e^{-\kappa l}(\kappa L+1) + \lambda\frac{2m}{\kappa^2\hbar^2}(\kappa L+1)e^{-\kappa l} & 1+2e^{-2\kappa l} + \lambda\frac{2m}{\kappa^2\hbar^2}\end{pmatrix} = 0$$

долго подумав над решением этого, мы приходим к ответу:

$$\lambda_1 = \frac{-\hbar^2\kappa^2}{2m}(1 + 2e^{-\kappa l}); \lambda_2 = \frac{-\hbar^2\kappa^2}{2m}(1 - 2e^{-\kappa l}).$$

пришли к успеху.

Б-2.2.18 Стенка и дельта-потенциал (!!!!!!!)

Частица массы m движется в одномерном потенциальном поле вида:

$$U(x) = \begin{cases} +\infty, & x < 0 \\ -A\delta(x-a), & x > 0 \end{cases}$$

Найти зависимость числа связанных состояний от параметров a и A.

Solution.

(???? давно хотел порешать, скоро сделаю это!!! По идее все, как и выше: назац, сшивка)
2.2.18. Единственное связанное состояние в яме существует при $\frac{mAa}{\hbar^2} > \frac{1}{2}$.

17.2.5 Problems about delta-potentials 2

Б-2.2.14 Вылет из δ-ямы при её внезапном ослаблении

Для частицы, находящейся в связанном состоянии в поле δ-ямы найти вероятность «ионизации» при внезапном изменении параметра ямы от $\varkappa_0$ до $\varkappa_1$.

Solution.

Вероятность остаться дается произведением волновых функций, которые известны, а, зная её, очевидна вероятность улететь.

$\psi(x) = \sqrt{\varkappa}\exp(-\varkappa|x|)$,

$$p = |\psi_{\varkappa_1}(x)\psi_{\varkappa_0}(x)|^2 = \left[\int\limits_{-\infty}^{+\infty} \sqrt{\varkappa_1\varkappa_0}e^{-(\varkappa_1+\varkappa_0)|x|}dx\right]^2 = \frac{4\sqrt{\varkappa_1\varkappa_0}}{\varkappa_1\varkappa_0}$$

Тогда вероятность электрона улететь равна

$$W_i = 1 - \frac{4\varkappa_0\varkappa_1}{(\varkappa_0+\varkappa_1)^2} = \left(\frac{\varkappa_0-\varkappa_1}{\varkappa_0+\varkappa_1}\right)^2.$$

Solution. через нахождение вне ямы (????)

(??? а через вероятности быть вне ямы можно было бы решить??? подумаю когда-то)

Б-2.2.15 Прохождение через δ-потенциал

Частица массы m свободно движется вдоль оси x с энергией E и попадает в область действия δ-потенциала. Найти коэффициенты прохождения и отражения, нарисовать графики.

Solution.

(?? вроде особых проблем не должно быть, потом потренируюсь.)
$R = \frac{\varkappa_0^2}{\varkappa_0^2+k^2}$, $\quad D = \frac{k^2}{\varkappa_0^2+k^2}$, где $E = \frac{\hbar^2k^2}{2m} > 0$.
(??? видимо, обозначения для $\varkappa_0$ из задачи вше.)

Ф1-29. Дираковская потенциальная гребенка

Solution.

(?? мб это про Кронинга-Пенни, открою когда-то еще раз)

МФТИ. Двигающиеся дельта-потенциалы (??)

Solution.

Вроде тут преобразование Галилея используется.
вывод его уже я писал, сюда переставлю

ПТФ-5.пр.1 Ионизация δ-ямы

Рассмотрим мелкую 1D яму под действием периодического электрического поля:

$$H = \frac{p^4}{2m} - \frac{\kappa}{m}\delta(x) + e\mathcal{E}x\cos\omega t.$$

Пусть частица находилась в основном состоянии; найдите частоту переходов в состояния непрерывного спектра в однофотонном приближении.

Solution.

Применяем правило Ферми.

$\hat{V} = \psi_i(x) = \sqrt{\kappa}e^{-\kappa|x|}$, переходы будут только в нечётные состояния непрерывного спектра $\psi_k^{(-)}(x) = \sin kx$,

$$F_{fi} = 2e\mathcal{E}\frac{k\kappa^{3/2}}{\left(\kappa^2+k^2\right)^2}$$

(??? этот ответ в другой задаче получен, допишу потом словами ходы для него!)

С учётом плотности состояний $d\nu_f = dk/\pi$, непосредственное применение золотого правила Ферми в таком случае даёт:

$$\frac{1}{\tau} = \int\limits_0^\infty 2\pi|F_{fi}|^2\delta\left(\frac{k^2+\kappa^2}{2m} - \omega\right)\frac{dk}{\pi} = \frac{2e^2\mathcal{E}^2}{m}\cdot\frac{E_0^{3/2}\sqrt{\omega-E_0}}{\omega^4}$$

(тут учтено, что член $+h\omega$, отвечающий испусканию фотона, отсутствует (???))

Б-2.2.19 δ-потенциал через функцию Грина

Найти функцию Грина $G(x,x')$ уравнения Шредингера для свободной частицы при $E < 0$ в одномерном случае. Используя эту функцию, найти энергию связанного состояния частицы в поле

$$U(x) = -\frac{\hbar^2}{m}\varkappa_0\delta(x).$$

Solution.

Функция Грина известна из теории, в рамках этого формализма для дельта-функции интеграл, дающий волновую функцию решается сразу.

$$G(x,x'): \qquad (\hat{\mathrm{H}} - E)G(x,x') = \left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - E\right\}G(x,x') = \delta(x-x').$$

$$\delta(x-x') = \int\frac{dk}{2\pi}e^{ik(x-x')}, \quad G(x,x') = \int\frac{dk}{2\pi}\widetilde{G}(k)e^{ik(x-x')}.$$

Подставляя эти разложения в (1), находим ($p = \hbar k, E = -|E| < 0$)

$$\tilde{G}(k) = \frac{1}{\frac{\hbar^2k^2}{2m} + |E|} = \frac{2m}{\hbar^2}\frac{1}{k^2+\varkappa^2} \qquad \varkappa^2 := 2m|E|/\hbar^2$$

$$G(x,x') = \frac{m}{\pi\hbar^2}\int\limits_{-\infty}^{\infty}dk\frac{e^{ik(x-x')}}{k^2+\varkappa^2} = \frac{m}{\hbar^2\varkappa}e^{-\varkappa|x-x'|}.$$

Интеграл вычисляется вычетами, нужно учитывать, что при $x - x' > 0$ контур интегрирования следует замыкать в верхней, а при $x - x' < 0$ - в нижней полуплоскости.

Общее решение уравнения Шредингера при $U(x) \neq 0, E < 0$ с учетом граничных условий при $x \to \pm\infty$ будет выглядеть так:

$$\psi(x) = -\frac{m}{\hbar^2 \varkappa} \int\limits_{-\infty}^{\infty} e^{-\varkappa|x-x'|} U(x') \psi(x') \, dx',$$

выбор $U(x) = -\hbar^2 \varkappa_0 \delta(x)/m$ приводит к результату задачи 2.2.6.
(напишу его)

17.2.6 Problems about oscillator 1

ПТФ-5.пр.1 Возбуждение осциллятора при $U = -F\hat{x}e^{-t^2}$

Найти вероятность перехода в первое и второе возбуждённые состояния гармонического осциллятора под действием силы, которая действует в течении конечного времени:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2} - F\hat{x}e^{-t^2/\tau^2},$$

если, при $t \to -\infty$ мы находились в основном состоянии осциллятора $|i\rangle = |0\rangle$;

Solution. для первого состояния

Решаем через правило Ферми.
Найдем $V_{nm}(t)$:

$$V_{nm}(t) = -Fe^{-t^2/\tau^2}\langle n|\hat{x}|m\rangle = -\frac{Fe^{-t^2/\tau^2}}{\sqrt{2m\omega}} \cdot \begin{cases} \sqrt{n}, & m = n-1 \\ \sqrt{n+1}, & m = n+1, \end{cases}$$

отличны от нуля только переходы между соседними уровнями.

$$w_{0\to1} = |-\frac{F}{\sqrt{2m\omega}} \int\limits_{-\infty}^{\infty} e^{-t^2/\tau^2} e^{i\omega t} dt|^2 = \frac{\pi F^2 \tau^2}{2m\omega} e^{-\omega^2\tau^2/2}$$

где $\omega_{10} = \omega$ - разница энергий.
Требуя малость поправки, мы приходим к выводу, что теория возмущений работает по параметру $F^2\tau^2/m\omega \ll 1$ либо $\omega\tau \gg 1$

Solution. для второго состояния

Чтобы найти вероятность перехода во второе возбуждённое состояние, нужно решить уравнение $i\frac{\partial\psi_n}{\partial t} = \sum\limits_m V_{nm}^{(I)}(t)\psi_m(t)$ точнее, а именно, во 2-м порядке ТВ:

$$\partial_t \psi_2^{(2)}(t) = -i \int\limits_{-\infty}^{t} d\tau_1 V_{21}^{(I)}(\tau_1) \psi_1^{(1)}(\tau_1) = (-i)^2 \int\limits_{-\infty}^{t} d\tau_1 V_{21}^{(I)}(\tau_1) \int\limits_{-\infty}^{\tau_1} d\tau_2 V_{10}^{(I)}(\tau_2)$$

$$w_{0\to2} = |\int\limits_{-\infty}^{\infty} d\tau_1 V_{21}(\tau_1) e^{i\omega\tau_1} \int\limits_{-\infty}^{\tau_1} d\tau_2 V_{10}(\tau_2) e^{i\omega\tau_2}|^2 =$$

$$= \frac{2F^4}{(2m\omega)^2} |\int\limits_{-\infty}^{\infty} d\tau_1 e^{-\tau_1^2/\tau^2 + i\omega\tau_1} \int\limits_{-\infty}^{\tau_1} d\tau_2 e^{-\tau_2^2/\tau^2 + i\omega\tau_2}|^2$$

(?? ниже хз, вообще нет идей, почему это так???)
Можно заметить, что стоящий тут интеграл равен половине такого же интеграла, но с бесконечными пределами $\int\limits_{-\infty}^{\infty} d\tau_1 \int\limits_{-\infty}^{\infty} d\tau_2$ благодаря чему мы можем сразу выписать для него результат:

$$w_{0\to2} = \frac{\pi^2 F^4 \tau^4}{8m^2\omega^2} e^{-\omega^2\tau^2}$$

Полученный результат оказался параметрически меньше $w_{0\to1}$, поскольку он связан со вторым порядком теории возмущений.

ПТФ-6.у2. Квантовый гармонический осциллятор (10 б)

• Вычислите $\langle \hat{x}^4 \rangle$ по произвольному собственному состоянию гармонического осциллятора $|n\rangle$.
• Частица находилась в основном состоянии гармонического осциллятора с частотой ω. Пусть в какой-то момент времени характерная частота осциллятора мгновенно меняется и становится равной ω'. Вычислите вероятность остаться в основном состоянии.

Solution.

• Действие операторов повышения и понижения:

$$\hat{a}|n\rangle = \sqrt{n}|n\rangle, \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n\rangle$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger)$$

$$\langle x^4 \rangle = \langle n|\hat{x}^4|n\rangle = \frac{\hbar^2}{4m^2\omega^2}\langle n|(\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + (\hat{a}^\dagger)^2)^2|n\rangle = \frac{\hbar^2}{4m^2\omega^2}\langle n|\hat{a}^4 + \hat{a}^3\hat{a}^\dagger + \hat{a}^2\hat{a}^\dagger\hat{a} +$$
$$+ \hat{a}^2(\hat{a}^\dagger)^2 + \hat{a}\hat{a}^\dagger\hat{a}^2 + \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \hat{a}(\hat{a}^\dagger)^2\hat{a} + \hat{a}(\hat{a}^\dagger)^3 + \hat{a}^\dagger\hat{a}^3 + \hat{a}^\dagger\hat{a}^2\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}(\hat{a}^\dagger)^2 + (\hat{a}^\dagger)^2\hat{a}^2 +$$
$$+ (\hat{a}^\dagger)^2\hat{a}\hat{a}^\dagger + (\hat{a}^\dagger)^3\hat{a} + (\hat{a}^\dagger)^4|n\rangle = \frac{\hbar^2}{4m^2\omega^2}((n+1)(n+2) + (n+1)^2 + n(n+1) + n(n+1) + n^2 + n(n-1))$$

$$\langle x^4 \rangle = \frac{3\hbar^2}{4m^2\omega^2}(2n^2 + 2n + 1)$$

• Волновая функция основного состояния:

$$\psi(x) = \sqrt[4]{\frac{m\omega}{\pi\hbar}} \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

$$P = \left|\int_{-\infty}^{\infty} \psi^*(x)\psi'(x)dx\right|^2 = \left|\sqrt[4]{\frac{m^2\omega\omega'}{\pi^2\hbar^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{m(\omega+\omega')x^2}{2\hbar}\right) dx\right|^2$$

$$P = \frac{2\sqrt{\omega\omega'}}{\omega + \omega'}$$

ПТФ-6.у3. Когерентные состояния

Когерентные состояния гармонического осциллятора определяются как собственные состояния для понижающего оператора $\hat{a}$ с собственным комплексным числом $\alpha \in \mathbb{C} : \hat{a}|\alpha\rangle = \alpha|\alpha\rangle$.
• Найдите координатное представление когерентного состояния $\psi_\alpha(x) \equiv \langle x|\alpha\rangle$. Для гамильтониана квантового гармонического осциллятора $\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})$, найдите также $\psi_\alpha(x,t) \equiv \langle x|\alpha(t)\rangle$.
• Выразите когерентное состояние α явно через собственные состояния осциллятора, нормировав его условием $\langle 0|\alpha\rangle = 1$.
• Представьте их в виде $|\alpha\rangle = \hat{C}(\alpha)|0\rangle$; найдите явный вид оператора $\hat{C}(\alpha)$.
• Вычислите перекрытие когерентных состояний $\langle\alpha|\alpha'\rangle$.
• Когерентные состояния образуют *переполненный базис*. Докажите следующую формулу для разложения единицы:

$$\hat{\mathbb{I}} = \int \frac{d\alpha d\alpha^*}{\pi} e^{-|\alpha|^2} |\alpha\rangle\langle\alpha|$$

(мы определили $d\alpha d\alpha^* \equiv d(\mathrm{Re}\alpha)d(\mathrm{Im}\alpha)$).

Solution.

• Оператор уничтожения:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2\hbar m\omega}}\hat{p}$$
$$\langle x|\hat{a}|\alpha\rangle = \alpha\langle x|\alpha\rangle = \alpha\psi_\alpha(x)$$

$$\left(\sqrt{\frac{m\omega}{2\hbar}}\hat{x}+\frac{i}{\sqrt{2\hbar m\omega}}\hat{p}\right)\psi_\alpha(x)=\alpha\psi_\alpha(x)$$

$$\left(\sqrt{\frac{m\omega}{2\hbar}}x+\sqrt{\frac{\hbar}{2m\omega}}\frac{\partial}{\partial x}\right)\psi_\alpha(x)=\alpha\psi_\alpha(x)$$

$$\sqrt{\frac{\hbar}{2m\omega}}\frac{\partial\psi_\alpha(x)}{\partial x}=\left(\alpha-\sqrt{\frac{m\omega}{2\hbar}}x\right)\psi_\alpha(x)$$

$$\psi_\alpha(x)=e^{\sqrt{\frac{2m\omega}{\hbar}}\alpha x-\frac{m\omega x^2}{2\hbar}}$$

Действие оператора эволюции (воспользуемся п. 2 этой задачи):

$$|\alpha,t\rangle=\hat{U}(t)|\alpha\rangle=\sum_n\frac{\alpha^n}{\sqrt{n!}}e^{-\frac{iE_nt}{\hbar}}|n\rangle$$

$$E_n=\hbar\omega\left(\frac{1}{2}+n\right)$$

$$|\alpha,t\rangle=e^{-\frac{i\omega t}{2}}\sum_n\frac{\alpha^n}{\sqrt{n!}}e^{-i\omega nt}|n\rangle=e^{-\frac{i\omega t}{2}}\sum_n\frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}}|n\rangle$$

$$\psi_\alpha(x,t)\equiv\langle x|\alpha(t)\rangle=e^{-\frac{i\omega t}{2}}\sum_n\frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}}\langle x|n\rangle$$

$$\psi_\alpha(x,t)=e^{-\frac{i\omega t}{2}}\sum_n\frac{(\alpha e^{-i\omega t})^n}{\sqrt{2^nn!}}\sqrt[4]{\frac{m\omega}{\pi\hbar}}H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right)$$

- Разложим когеренстное состояние по базису:

$$|\alpha\rangle=\sum_n C_n(\alpha)|n\rangle,\quad C_n(\alpha)=\langle n|\alpha\rangle=\frac{1}{\alpha}\langle n|\hat{a}\alpha\rangle=\frac{1}{\alpha}\langle\hat{a}^\dagger n|\alpha\rangle$$

$$\hat{a}^\dagger|n\rangle=\sqrt{n+1}|n+1\rangle$$

Получаем рекуррентное соотношение:

$$\alpha C_n(\alpha)=\sqrt{n+1}C_{n+1}(\alpha)\to C_n(\alpha)=\frac{\alpha^n}{\sqrt{n!}}C_0(\alpha)$$

Условие нормировки:

$$C_0(\alpha)=\langle 0|\alpha\rangle=1$$

$$|\alpha\rangle=\sum_n\frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

$$|n\rangle=\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle$$

$$|\alpha\rangle=\sum_n\frac{(\alpha a^\dagger)^n}{n!}|0\rangle=e^{\alpha\hat{a}^\dagger}|0\rangle=C(\alpha)|0\rangle$$

$$C(\alpha)=e^{\alpha\hat{a}^\dagger}$$

$$\langle\alpha|\alpha'\rangle=\langle 0|\hat{C}^\dagger(\alpha)\hat{C}(\alpha')|0\rangle=\langle 0|e^{\alpha^*\hat{a}}e^{\alpha'\hat{a}^\dagger}|0\rangle=\left\langle 0\left|\sum_{k=0}^\infty\frac{(\alpha^*\hat{a})^k}{k!}\sum_{n=0}^\infty\frac{(\alpha'\hat{a}^\dagger)^n}{n!}\right|0\right\rangle=$$

$$=\left\langle k\left|\sum_{k=0}^\infty\frac{\hat{a}^k}{\sqrt{k!}}\sum_{n=0}^\infty\frac{\alpha'^n}{\sqrt{n!}}\right|n\right\rangle=\sum_{k=0}^\infty\frac{(\alpha^*)^k}{\sqrt{k!}}\sum_{n=0}^\infty\frac{(\alpha')^n}{\sqrt{n!}}\delta_{kn}=\sum_{n=0}^\infty\frac{(\alpha^*\alpha')^n}{n!}=e^{\alpha^*\alpha'}$$

$$\langle\alpha|\alpha'\rangle=e^{\alpha^*\alpha'}$$

- $$\langle m|\hat{\mathbb{I}}|n\rangle=\delta_{mn}$$

$$\left\langle m \left| \int \frac{d\alpha d\alpha^*}{\pi} e^{-|\alpha|^2} |\alpha\rangle\langle\alpha| \right| n \right\rangle = \int \frac{d\alpha d\alpha^*}{\pi} e^{-|\alpha|^2} \langle m|\alpha\rangle\langle\alpha|n\rangle = \int \frac{d\alpha d\alpha^*}{\pi} e^{-|\alpha|^2} \frac{(\alpha^*)^m}{\sqrt{m!}} \frac{\alpha^n}{\sqrt{n!}}$$

$$\alpha = re^{i\varphi}, \qquad d(\mathrm{Re}\alpha)d(\mathrm{Im}\alpha) = rdrd\varphi$$

$$\int_0^\infty \int_0^{2\pi} \frac{drd\varphi}{\pi} re^{-r^2} \frac{r^{m+n}e^{i(n-m)\varphi}}{\sqrt{m!n!}} = \frac{1}{\sqrt{m!n!}} \int_0^\infty drr^{m+n+1}e^{-r^2} \int_0^{2\pi} \frac{d\varphi}{\pi} e^{i(n-m)\varphi} =$$

$$= \frac{2}{\sqrt{m!n!}} \int_0^\infty drr^{m+n+1}e^{-r^2}\delta_{nm} = \frac{1}{m!} \int_0^\infty d(r^2)r^{2m}e^{-r^2}\delta_{mn} = \frac{\Gamma(m+1)}{m!}\delta_{mn} = \delta_{mn}$$

Таким образом,

$$\hat{\mathbb{I}} = \int \frac{d\alpha d\alpha^*}{\pi} e^{-|\alpha|^2} |\alpha\rangle\langle\alpha|$$

ПТФ-6.з1. Теорема Вика

Квантовый гармонический осциллятор находится при температуре T, т.е. описывается матрицей плотности $\hat{\rho} = \frac{1}{Z}e^{-\beta\omega\hat{a}^\dagger\hat{a}}$. Вычислите среднее значение по этому состоянию от оператора $\langle e^{\alpha_1\hat{a}+\alpha_2\hat{a}^\dagger}\rangle$ и докажите следующее соотношение:

$$\langle e^{\alpha_1\hat{a}+\alpha_2\hat{a}^\dagger}\rangle = e^{\frac{1}{2}\langle(\alpha_1\hat{a}+\alpha_2\hat{a}^\dagger)^2\rangle}$$

Указание: вам может пригодиться базис когерентных состояний, а также формула Бейкера-Кэмбелла-Хаусдорфа:

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\frac{1}{2}[\hat{A},\hat{B}]}, \quad [\hat{A},[\hat{A},\hat{B}]] = [\hat{B},[\hat{A},\hat{B}]] = 0$$

Solution.

Рассмотрим $\hat{O} = e^{\alpha_1\hat{a}+\alpha_2\hat{a}^\dagger}$.

$$\langle\hat{O}\rangle = \mathrm{Tr}(\hat{\rho}\hat{O}) = \mathrm{Tr}\left(\frac{1}{Z}e^{-\beta\omega\hat{a}^\dagger\hat{a}}e^{\alpha_1\hat{a}+\alpha_2\hat{a}^\dagger}\right)$$

$$\langle\hat{O}\rangle = \mathrm{Tr}\left(\frac{1}{Z}e^{-\beta\omega\hat{a}^\dagger\hat{a}}e^{\alpha_1\hat{a}+\alpha_2\hat{a}^\dagger}\right) = \frac{1}{Z}\int \frac{d\alpha d\alpha^*}{\pi} e^{-|\alpha|^2}\langle\alpha|e^{\alpha_1\hat{a}+\alpha_2\hat{a}^\dagger}e^{-\beta\omega\hat{a}^\dagger\hat{a}}|\alpha\rangle$$

$$e^{\alpha_1\hat{a}+\alpha_2\hat{a}^\dagger} = e^{\alpha_1\hat{a}}e^{\alpha_2\hat{a}^\dagger}e^{-\frac{\alpha_1\alpha_2}{2}[\hat{a}^\dagger,\hat{a}]} = e^{\alpha_1\hat{a}}e^{\alpha_2\hat{a}^\dagger}e^{\frac{\alpha_1\alpha_2}{2}}$$

$$\langle\hat{O}\rangle = \frac{1}{Z}\int \frac{d\alpha d\alpha^*}{\pi} e^{-|\alpha|^2}e^{\alpha_2\alpha^*}e^{\frac{\alpha_1\alpha_2}{2}}\langle\alpha|e^{\alpha_1\hat{a}}e^{-\beta\omega\hat{a}^\dagger\hat{a}}|\alpha\rangle$$

$$e^{-\beta\omega\hat{a}^\dagger\hat{a}}|\alpha\rangle = e^{-\beta\omega\hat{a}^\dagger\hat{a}}\sum_{n=0}^\infty \frac{\alpha^n}{\sqrt{n!}}|n\rangle = \sum_{n=0}^\infty \frac{\alpha^n}{\sqrt{n!}}e^{-\beta\omega n}|n\rangle = e^{-\beta\omega}|n\rangle$$

$$\langle\hat{O}\rangle = \frac{e^{\frac{\alpha_1\alpha_2}{2}}}{Z}\int \frac{d\alpha d\alpha^*}{\pi} e^{-|\alpha|^2}e^{\alpha_2\alpha^*}e^{\alpha_1\alpha e^{-\beta\omega}}\langle\alpha|e^{-\beta\omega}|\alpha\rangle =$$

$$= \frac{e^{\frac{\alpha_1\alpha_2}{2}}}{Z}\int \frac{d\alpha d\alpha^*}{\pi} e^{-|\alpha|^2(1-e^{-\beta\omega})}e^{\alpha_2\alpha^*}e^{\alpha_1\alpha e^{-\beta\omega}}$$

$$\langle\hat{O}\rangle = \frac{e^{\frac{\alpha_1\alpha_2}{2}}}{Z}(1-e^{-\beta\omega})\int_{-\infty}^\infty \frac{du}{\sqrt{\pi}} e^{-(u^2-\frac{\alpha_2+\alpha_1e^{-\beta\omega}}{\sqrt{1-e^{-\beta\omega}}}u)} \int_{-\infty}^\infty \frac{du}{\sqrt{\pi}} e^{-(u^2+i\frac{\alpha_2-\alpha_1e^{-\beta\omega}}{\sqrt{1-e^{-\beta\omega}}}u)}$$

$$Z = \mathrm{Tr}(e^{-\beta\omega\hat{a}^\dagger\hat{a}}) = \sum_{n=0}^\infty \langle n|e^{-\beta\omega\hat{a}^\dagger\hat{a}}|n\rangle = \sum_{n=0}^\infty \langle n|e^{-\beta\omega n}|n\rangle = \sum_{n=0}^\infty e^{-\beta\omega n} = \frac{1}{1-e^{-\beta\omega}}$$

$$\langle\hat{O}\rangle = e^{\frac{\alpha_1\alpha_2}{2}}e^{\frac{(\alpha_2+\alpha_1e^{-\beta\omega})^2}{4(1-e^{-\beta\omega})}}e^{-\frac{(\alpha_2-\alpha_1e^{-\beta\omega})^2}{4(1-e^{-\beta\omega})}} = e^{\frac{\alpha_1\alpha_2}{2}\left(\frac{1+e^{-\beta\omega}}{1-e^{-\beta\omega}}\right)}$$

$$\langle e^{\alpha_1\hat{a}+\alpha_2\hat{a}^\dagger}\rangle = e^{\frac{\alpha_1\alpha_2}{2}\coth\frac{\beta\omega}{2}}$$

Рассмотрим $\hat{O} = (\alpha_1\hat{a} + \alpha_2\hat{a}^\dagger)^2$.

$$\begin{aligned}
\langle\hat{O}\rangle &= \mathrm{Tr}(\hat{\rho}\hat{O}) = \mathrm{Tr}\left(\frac{1}{Z}e^{-\beta\omega\hat{a}^\dagger\hat{a}}(\alpha_1\hat{a}+\alpha_2\hat{a}^\dagger)^2\right) = \\
&= \sum_{n=0}^{\infty}\left\langle n\left|\frac{1}{Z}e^{-\beta\omega\hat{a}^\dagger\hat{a}}(\alpha_1\hat{a}+\alpha_2\hat{a}^\dagger)^2\right|n\right\rangle = \\
&= \frac{1}{Z}\sum_{n=0}^{\infty}\left\langle n\left|\frac{1}{Z}e^{-\beta\omega\hat{a}^\dagger\hat{a}}(\alpha_1^2\hat{a}^2+\alpha_1\alpha_2\hat{a}\hat{a}^\dagger+\alpha_1\alpha_2\hat{a}^\dagger\hat{a}+\alpha_2^2\hat{a}^{\dagger 2})\right|n\right\rangle = \\
&= \frac{\alpha_1\alpha_2}{Z}\sum_{n=0}^{\infty}\langle n|e^{-\beta\omega\hat{a}^\dagger\hat{a}}(2n+1)|n\rangle = \\
&= \frac{\alpha_1\alpha_2}{Z}\sum_{n=0}^{\infty}e^{-\beta\omega n}(2n+1) = \frac{\alpha_1\alpha_2}{Z}\frac{1+e^{-\beta\omega}}{(1-e^{-\beta\omega})^2} = \\
&= \alpha_1\alpha_2\frac{1+e^{-\beta\omega}}{1-e^{-\beta\omega}} = \alpha_1\alpha_2\coth\frac{\beta\omega}{2}
\end{aligned}$$

$$e^{\frac{1}{2}\langle(\alpha_1\hat{a}+\alpha_2\hat{a}^\dagger)^2\rangle} = e^{\frac{\alpha_1\alpha_2}{2}\coth\frac{\beta\omega}{2}} = \langle e^{\alpha_1\hat{a}+\alpha_2\hat{a}^\dagger}\rangle$$

Таким образом, теорема Вика доказана.

ПТФ-6.з2. Oscillator in a box

Квантовый гармонический осциллятор помещён в большую коробку размера $2L$ ровно посередине:

$$U(x) = \begin{cases}\frac{m\omega^2x^2}{2}, & |x| < L\\ \infty, & |x| > L\end{cases}$$

Определите *силу*, с которой осциллятор, находясь в одном из низколежащих уровней энергии $n \ll \frac{m\omega L^2}{\hbar}$, действует на эти стенки.

Solution.

Мы знаем общее решение, нужно подставить граничные условия и получить условие на поправку к энергии. (??? как догадаться про матем преобразования тут??? это еще в 1 части указывать буду!)

Общее решение в области $|x| < L$:

$$\psi(y) = C_1{}_1F_1\left(-\frac{\varepsilon}{2},\frac{1}{2},y^2\right)e^{-\frac{y^2}{2}} + C_2y_1F_1\left(-\frac{\varepsilon-1}{2},\frac{3}{2},y^2\right)e^{-\frac{y^2}{2}} = C_1\psi_1(y) + C_2\psi_2(y)$$

$$x_\pm := \pm L \qquad \Rightarrow \qquad y := \pm L\sqrt{\frac{m\omega}{\hbar}}$$

$$\psi\left(\pm L\sqrt{\frac{m\omega}{\hbar}}\right) = 0$$

First we consider the first part of ψ:

$${}_1F_1\left(-\frac{\varepsilon}{2},\frac{1}{2},y^2\right)e^{-\frac{m\omega L^2}{\hbar}} = 0$$

Поскольку $\frac{m\omega L^2}{\hbar} \gg 1$, то воспользуемся ${}_1F_1(a,b,z) \approx \frac{\Gamma(b)}{\Gamma(a)}e^zz^{a-b} + \frac{\Gamma(b)}{\Gamma(b-a)}(-z)^{-a}$:

$$\frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(-\frac{\varepsilon}{2}\right)}e^zz^{-\frac{\varepsilon+1}{2}} + \frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{\varepsilon+1}{2}\right)}(-z)^{\frac{\varepsilon}{2}} = 0$$

$$e^z + \frac{\Gamma(-\frac{\varepsilon}{2})}{\Gamma(\frac{\varepsilon+1}{2})}(-1)^{\frac{\varepsilon}{2}}z^{\varepsilon+\frac{1}{2}} = 0$$

Here we have:

$$\Gamma\left(-\frac{\varepsilon}{2}\right)\Gamma\left(1+\frac{\varepsilon}{2}\right)=\frac{\pi}{\sin\left(-\frac{\pi\varepsilon}{2}\right)}$$

$$\frac{\Gamma\left(-\frac{\varepsilon}{2}\right)}{\Gamma\left(\frac{\varepsilon+1}{2}\right)}=-\frac{\pi}{\sin\frac{\pi\varepsilon}{2}\Gamma\left(1+\frac{\varepsilon}{2}\right)\Gamma\left(\frac{1+\varepsilon}{2}\right)}=-\frac{2^{\varepsilon}\sqrt{\pi}}{\sin\frac{\pi\varepsilon}{2}\Gamma(1+\varepsilon)}=-\frac{2^{\varepsilon}\sqrt{\pi}}{\sin\frac{\pi\varepsilon}{2}\varepsilon\Gamma(\varepsilon)}$$

because $\Gamma(z)\Gamma\left(z+\frac{1}{2}\right)=2^{1-2z}\sqrt{\pi}\Gamma(2z)$;

$$\Gamma(\varepsilon)=\Gamma(n+\delta n)=(n-1+\delta n)...(1+\delta n)\Gamma(1+\delta n)\approx\Gamma(n)$$

(??? почему эпсилон так от н зависит и какой смысл в вариации н?? это важная часть метода!!! впишу в 1ю про это?)

$$\frac{\Gamma\left(-\frac{\varepsilon}{2}\right)}{\Gamma\left(\frac{\varepsilon+1}{2}\right)}=-\frac{2^{n}\sqrt{\pi}}{\sin(\frac{\pi n}{2}+\frac{\pi\delta n}{2})n\Gamma(n)\Gamma(1+\delta n)}\approx\begin{cases}-\frac{(-1)^{k}2^{n}\sqrt{\pi}}{n\Gamma(n)}, & n=2k+1\\ -\frac{(-1)^{k}2^{n+1}}{\sqrt{\pi}n\delta n\Gamma(n)}, & n=2k\end{cases}$$

and we can substitute it:

$$e^{z}-\frac{2^{n+1}\sqrt{\pi}}{\pi\delta nn\Gamma(n)}z^{n+\frac{1}{2}}=0\quad(n=2k)$$

$$\delta n=\frac{e^{-z}2^{n+1}}{\sqrt{\pi}n\Gamma(n)}z^{n+\frac{1}{2}}$$

Now, the second part and apply the same algorithm:

$${}_1F_1\left(-\frac{\varepsilon-1}{2},\frac{3}{2},\frac{m\omega L^2}{\hbar}\right)e^{-\frac{m\omega L^2}{2\hbar}}=0$$

$$\frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(-\frac{\varepsilon-1}{2}\right)}e^{z}z^{-\frac{\varepsilon}{2}-1}+\frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{\varepsilon+1}{2}\right)}(-z)^{\frac{\varepsilon-1}{2}}=0$$

$$e^{z}+\frac{\Gamma\left(-\frac{\varepsilon-1}{2}\right)}{\Gamma\left(1+\frac{\varepsilon}{2}\right)}(-1)^{\frac{\varepsilon+1}{2}}z^{\varepsilon+\frac{1}{2}}=0$$

$$\Gamma\left(-\frac{\varepsilon-1}{2}\right)\Gamma\left(\frac{\varepsilon+1}{2}\right)=\frac{\pi}{\sin\left(-\frac{\pi(\varepsilon-1)}{2}\right)}$$

$$\frac{\Gamma\left(-\frac{\varepsilon-1}{2}\right)}{\Gamma\left(1+\frac{\varepsilon}{2}\right)}=-\frac{\pi}{\sin\left(\frac{\pi(\varepsilon-1)}{2}\right)\Gamma\left(\frac{\varepsilon}{2}+1\right)\Gamma\left(\frac{1+\varepsilon}{2}\right)}=-\frac{\pi}{\sqrt{\pi}2^{-\varepsilon}\varepsilon\Gamma(\varepsilon)\sin\left(\frac{\pi(\varepsilon-1)}{2}\right)}=$$

$$=-\frac{2^{\varepsilon}\sqrt{\pi}}{\sin\left(\frac{\pi}{2}(n-1)+\frac{\pi}{2}\delta n\right)n\Gamma(n)}\approx\begin{cases}\frac{(-1)^{k}2^{\varepsilon}\sqrt{\pi}}{n\Gamma(n)}, & n=2k+1\\ \frac{(-1)^{k}2^{\varepsilon+1}}{\sqrt{\pi}n\delta n\Gamma(n)}, & n=2k\end{cases}$$

$$e^{z}-\frac{2^{n+1}\sqrt{\pi}}{\pi\delta nn\Gamma(n)}z^{n+\frac{1}{2}}=0\quad(n=2k+1)$$

$$\delta n=\frac{e^{-z}2^{n+1}}{\sqrt{\pi}n\Gamma(n)}z^{n+\frac{1}{2}},$$

which is the same. Таким образом,

$$\forall n\in\mathbb{Z}\quad\delta n=e^{-\frac{m\omega L^2}{\hbar}}\left(\frac{m\omega L^2}{\hbar}\right)^{n+\frac{1}{2}}\frac{2^{n+1}}{\sqrt{\pi}\Gamma(n+1)}.$$

$$E_n=\hbar\omega\left(\frac{1}{2}+n+\frac{2^{n+1}e^{-\frac{m\omega L^2}{\hbar}}\left(\frac{m\omega L^2}{\hbar}\right)^{n+\frac{1}{2}}}{\sqrt{\pi}\Gamma(n+1)}\right)$$

$$F_n=-\frac{\partial E_n}{\partial L}\approx\frac{2^{n+2}m\omega^2Le^{-\frac{m\omega L^2}{\hbar}}\left(\frac{m\omega L^2}{\hbar}\right)^{n+\frac{1}{2}}}{\sqrt{\pi}\Gamma(n+1)}$$

Б-2.3.7.б) Oscillator near a wall

Найти энергетические уровни частицы, движущейся в потенциальном поле вида

$$V(x) = \begin{cases} \infty, & x \leqslant 0 \\ \frac{m\omega^2 x^2}{2}, & x > 0 \end{cases}$$

Solution.

б) $E'_n = E_{2n+1} = \hbar\omega(2n + 1 + 1/2) = 2\hbar\omega(n + 3/4)$.

Б-2.3.1 Импульсы основного состояния (???)

Найти распределение по импульсам для основного состояния гармонического осциллятора.

Solution.

(волновую функцию в импульсном представлении, то есть преобразование фурье сделать от нее в координатном??)

Б-2.3.2 Средние x^2 и p^2

Для одномерного гармонического осциллятора вычислить $\langle n|\hat{\mathrm{x}}^2|n\rangle$, $\langle n|\hat{\mathrm{p}}^2|n\rangle$ и сравнить с классическим результатом для x^2 и p^2.

Solution.

Воспользуемся выражениями

$$\hat{x} = \frac{x_0}{\sqrt{2}}\left(\hat{a}^+ + \hat{a}\right), \quad \hat{\mathrm{p}} = i\frac{p_0}{\sqrt{2}}\left(\hat{a}^+ - \hat{a}\right), \quad x_0 = \sqrt{\frac{\hbar}{m\omega}}, p_0 = \sqrt{\hbar m\omega}.$$

Тогда получим, что

$$\langle\hat{x}^2\rangle = \langle n|\hat{x}^2|n\rangle = \frac{x_0^2}{2}\langle n|\hat{a}^+\hat{a} + \hat{a}\hat{a}^+|n\rangle = x_0^2\left(n + \frac{1}{2}\right) = \frac{E_n}{m\omega^2},$$
$$\langle\hat{\mathrm{p}}^2\rangle = \langle n|\hat{\mathrm{p}}^2|n\rangle = \frac{p_0^2}{2}\langle n|\hat{a}^+\hat{a} + \hat{a}\hat{a}^+|n\rangle = p_0^2\left(n + \frac{1}{2}\right) = mE_n,$$

где $E_n = \hbar\omega(n + 1/2)$ - энергия квантового осциллятора.

Для классического осциллятора общее решение уравнений движения имеет вид

$$x_{\text{кл}} = A\sin(\omega t + \varphi), \quad p_{\text{кл}} = m\omega A\cos(\omega t + \varphi),$$

где A - амплитуда колебаний, а φ - начальная фаза. Нетрудно найти

$$\overline{x^2_{\text{cl}}} = \frac{1}{T}\int\limits_0^T A^2\sin^2(\omega t + \varphi)dt = \frac{A^2}{2} = \frac{E_{\text{K}}}{m\omega^2},$$
$$\overline{p^2_{\text{K}\Omega}} = (m\omega)^2\overline{x^2_{\text{K}}} = mE_{\text{K}\Omega}.$$

Согласно принципу соответствия в пределе $n \to \infty$ выражения для квантовых средних должны переходить в соответствующие выражения для классических средних для одного и того же значения энергии ($E_n = E_{\text{кл}}$). Для гармонического осциллятора данное равенство выполняется не только при $n \to \infty$, но и для любых n.

Б-2.3.3 Средние $\hat{x}^4$ и $\hat{x}^{2k+1}$

Воспользовавшись понижающим и повышающим операторами, $\hat{a}$ и $\hat{a}^+$, найдите средние значения операторов $\hat{x}^4$ и $\hat{x}^{2k+1}$ в n-м стационарном состоянии линейного гармонического осциллятора.

Solution.

(решается прямолинейно, ничего сложного)
Ответ: $\langle\hat{x}^4\rangle = \langle n|\hat{x}^4|n\rangle = \frac{x_0^4}{4}\left(6n^2+6n+3\right)$, $\langle\hat{x}^{2k+1}\rangle = \langle n|\hat{x}^{2k+1}|n\rangle = 0, \quad k = 0, 1, ...$

Б-2.3.4 Дисперсии в осцилляторе

Вычислить произведение дисперсий $\Delta\mathrm{p}\Delta\mathrm{x}$ для n-го состояния осциллятора.

Solution.

Можно дисперсии выразить через среднее значения, которые известно, как посчитать:

$$\Delta\mathrm{p}\Delta\mathrm{x} = \sqrt{\langle\Delta\mathrm{p}^2\rangle}\sqrt{\langle\Delta\mathrm{x}^2\rangle} = E_n/\omega = \hbar(n+1/2),$$

где

$$\langle\hat{x}^2\rangle = \langle n|\hat{x}^2|n\rangle = \frac{x_0^2}{2}\langle n|\hat{a}^+\hat{a}+\hat{a}\hat{a}^+|n\rangle = x_0^2\left(n+\frac{1}{2}\right) = \frac{E_n}{m\omega^2},$$
$$\langle\hat{\mathrm{p}}^2\rangle = \langle n|\hat{\mathrm{p}}^2|n\rangle = \frac{p_0^2}{2}\langle n|\hat{a}^+\hat{a}+\hat{a}\hat{a}^+|n\rangle = p_0^2\left(n+\frac{1}{2}\right) = mE_n,$$

Б-2.3.5

Найти для гармонического осциллятора $\hat{a}$ и $\hat{a}^+$в представлении Гейзенберга.

Solution.

2.3.5. $\hat{a}_H = \hat{a}\exp(-i\omega t), \hat{a}_H^+ = \hat{a}^+\exp(i\omega t)$. Использовать результат задачи 2.1.17.

Б-2.3.6

Вычислить $[\hat{a}, f(\hat{a}^+)]$, если $[\hat{a}, \hat{a}^+] = 1$.

Solution.

17.2.7 Problems about oscillator 2

Leuven.s5. Oscillator in linear potential

We consider a 1D harmonic oscillator perturbed by a small linear potential, i.e.

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 - \lambda\hat{x}$$

with $0 < \lambda \ll 1$.
(a) Compute the energy shift for a state $|n\rangle$ up to the first non-vanishing order.
(b) Find the exact solution to this problem and compare it to the pertubative solution.

Solution.

The main idea is to use time independent PT, it is an easy problem, can be done in 2-5 minutes.

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}+\hat{a}^\dagger\right), \quad \hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

$$V_{kn} = \langle k|\hat{V}|n\rangle = -\lambda\frac{\hbar}{2m\omega}\left(\sqrt{n}\delta_{k,n-1}+\sqrt{n+1}\delta_{k,n+1}\right)$$

$$\Delta_n^{(1)} = V_{nn} = 0,$$

$$\Delta_n^{(2)} = \sum_{k \neq n} \frac{|V_{kn}|^2}{E_n^{(0)} - E_k^{(0)}} = -\frac{\lambda^2}{2m\omega^2}$$

The analytical solution is obtained by $\hat{H} \equiv \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2(\hat{x} - \frac{\lambda}{m\omega^2})^2 - \frac{\lambda^2}{2m\omega^2}$. If we define $\hat{y}_\cdot = \left(\hat{x} - \frac{\lambda}{m\omega^2}\right)$, we see that difference in energy is $-\frac{\lambda^2}{2m\omega^2}$.

Б-2.3.7.а) Вне границ

Частица движется в потенциальном поле $V(x) = \frac{m\omega^2 x^2}{2}$. Определить вероятность нахождения частицы вне классических границ для основного состояния.

Solution.

По смыслу волновой функции сразу пишем ответ, нужно лишь размерности удобные подобрать.
Ответ: $w = \frac{\int_1^\infty e^{-y^2} dy}{\int_0^\infty e^{-y^2} dy} \simeq 0,16$.

Б-2.3.8 Импульсный осциллятор

Написать уравнение Шредингера для осциллятора в p-представлении и определить распределение вероятностей различных значений импульса.

Solution.

(???? тут не уверен, почему именно спецфункция Генкеля решает это? и какой график их???)
2.3.8. $\left(\frac{p^2}{2m} - \frac{m\omega^2\hbar^2}{2}\frac{d^2}{dp^2}\right)\phi_n(p) = E_n\phi_n(p)$

$$|\phi_n(p)|^2 dp = \frac{1}{2^n n!\sqrt{\pi}p_0} \exp\left[-\left(\frac{p}{p_0}\right)^2\right] H_n^2\left(\frac{p}{p_0}\right) dp.$$

Б-2.3.9

Для когерентного состояния осциллятора $|z\rangle$ показать, что

$$\frac{\langle z|\hat{\mathrm{H}}|z\rangle}{\langle z|z\rangle} = \hbar\omega\left(|z|^2 + 1/2\right),$$

где $\hat{\mathrm{H}}$ - гамильтониан гармонического осциллятора с частотой ω.

Solution.

(чет так я хз, как решать, но вроде это у нас как раз энергия, может какая-то теорема Фейнмана-Хеллмана поможет?)
2.3.9. Когерентное состояние $|z\rangle$ является собственным вектором оператора $\hat{a}$, отвечающим собственному значению z (комплексному). На основании этого имеем

$$\frac{\langle z|\hat{\mathrm{H}}|z\rangle}{\langle z|z\rangle} = \frac{\hbar\omega\langle z|\hat{a}^+\hat{a} + \frac{1}{2}|z\rangle}{\langle z|z\rangle} = \frac{\hbar\omega\langle z|z^*z + \frac{1}{2}|z\rangle}{\langle z|z\rangle} = \hbar\omega\left(|z|^2 + \frac{1}{2}\right).$$

Б-2.3.10

Для когерентного состояния осциллятора $|z(t)\rangle$ вычислить среднее значение операторов $\hat{\mathrm{x}}$ и $\hat{\mathrm{p}}$ и сравнить результат с классической траекторией в фазовом пространстве осциллятора.

Solution.

2.3.10. Эволюция во времени когерентного состояния определяется гамильтонианом гармонического осциллятора $\hat{\mathrm{H}} = \hbar\omega\left(\hat{a}^{+}\hat{a} + \frac{1}{2}\right)$, т. е. $|z(t)\rangle = \exp\left(-\frac{i}{\hbar}\hat{\mathrm{H}}t\right)|z(0)\rangle$. Это означает, что

$$\langle\hat{x}\rangle_t = \langle z(t)|\hat{x}|z(t)\rangle = \langle z(0)|e^{\frac{i}{\hbar}\hat{\mathrm{H}}t}\hat{x}e^{-\frac{i}{\hbar}\hat{\mathrm{H}}t}|z(0)\rangle = \langle z(0)|\hat{x}_H|z(0)\rangle,$$
$$\langle\hat{\mathrm{p}}\rangle_t = \langle z(t)|\hat{\mathrm{p}}|z(t)\rangle = \langle z(0)|\hat{\mathrm{p}}_H|z(0)\rangle.$$

где $\hat{x}_H, \hat{\mathrm{p}}_H$ - операторы координаты и импульса в гейзенберговском представлении (см. задачи 2.1.17 и 2.1.23). Несложный расчет приводит к результату $\begin{cases} \langle\hat{x}\rangle_t = \langle\hat{x}\rangle_0\cos\omega t + \frac{\langle\hat{\mathrm{p}}\rangle_0}{m\omega}\sin\omega t, \\ \langle\hat{\mathrm{p}}\rangle_t = \langle\hat{\mathrm{p}}\rangle_0\cos\omega t - m\omega\langle\hat{x}\rangle_0\sin\omega t, \end{cases}$ где $\begin{cases} \langle\hat{x}\rangle_0 = \langle z(0)|\hat{x}|z(0)\rangle, \\ \langle\hat{\mathrm{p}}\rangle_0 = \langle z(0)|\hat{\mathrm{p}}|z(0)\rangle. \end{cases}$

Таким образом, эволюция во времени средних значений координаты и импульса в когерентном состоянии квантового осциллятора в точности соответствует закону изменения координаты и импульса классического осциллятора при движении по классической траектории.

Б-2.3.11 Волновая функция когерентного состояния

Найти волновую функцию для когерентного состояния осциллятора $|z\rangle$ в координатном и импульсном представлении.

Solution.

2.3.11. Основное состояние гармонического осциллятора $|0\rangle$ представляет собой когерентное состояние с $z = 0$. Вектор состояния $|0\rangle$ onределяется из уравнения $\hat{a}|0\rangle = 0$ (см. (II.17)). После перехода к координатному представлению это уравнение принимает вид

$$\left(\xi + \frac{d}{d\xi}\right)\psi_0(\xi) = 0 \qquad \Rightarrow \qquad \psi_0(\xi) = Ce^{-\frac{\xi^2}{2}}.$$

(Использованы обозначения: $\xi = x/x_0, \psi_0(\xi) = \langle\xi|0\rangle$ - волновая функция основного состояния в координатном представлении.)

Уравнение для $\langle\xi|z\rangle$ - волновой функции когерентного состояния

$$\frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right)\langle\xi|z\rangle = z\langle\xi|z\rangle$$

является модификацией предыдущего уравнения с заменой $\xi \to \xi - \sqrt{2}z$. Поэтому искомая функция имеет вид

$$\langle\xi|z\rangle = C\exp\left[-\frac{1}{2}(\xi - \sqrt{2}z)^2\right].$$

В импульсном представлении по аналогии получаем

$$\langle p|z\rangle = C\exp\left[-\frac{1}{2}\left(\frac{p}{p_0} + \sqrt{2}z\right)^2\right].$$

Фактически обе функции являются собственными функциями основного состояния, “сдвинутыми" в комплексной плоскости на чнсло z.

Б-2.3.12

Заряженный гармонический осциллятор находится в основном состоянии в однородном электрическом поле $\mathcal{E}\|x$, которое внезапно выключается в момент времени $t = 0$. Определить вероятность обнаружить осциллятор на n-м возбужденном уровне энергии при $t > 0$.

2.3.12. Гамильтониан заряженного осциллятора в однородном электрическом поле (в системе единиц $m = 1, \hbar = 1$) имеет вид

$$\hat{\mathrm{H}} = \frac{\hat{\mathrm{p}}_x^2}{2} + \frac{\omega^2 x^2}{2} - e\varepsilon x.$$

Волновая функция основного состояния осциллятора с гамильтонианом (1) при $t < 0$ в осцилляторных единицах имеет вид

$$\psi(Q,t)|_{t<0} = e^{-iEt}\frac{1}{\pi^{1/4}}e^{-\frac{1}{2}(Q-e\varepsilon)^2}.$$

Сравнивая с когерентным состоянием (см. задачу 2.3.11), видим что в нашем случае параметр $z = e\mathcal{E}/\sqrt{2}$. Таким образом, вероятность обнаружить осциллятор в момент времени $t > 0$ на n-м возбужденном уровне энергии равна

$$w_{E_n} = \frac{(e\mathcal{E})^{2n}}{n!} e^{-(e\mathcal{E})^2}$$

в соответствии с (II.20).

Б-2.3.13

В когерентном состоянии гармонического осциллятора найти

$$\langle \Delta \hat{\mathrm{x}}^2 \rangle \langle \Delta \hat{\mathrm{p}}^2 \rangle.$$

ЛШ-6 Переходы в осцилляторе

Заряженная частица массы m движется по прямой в параболическом потенциале $U(x) = m\omega^2 x^2/2$. На короткое время τ включают слабое электрическое поле E, а затем выключают.

Какова вероятность перевести частицу в состояние $|n\rangle$, если до включения поля она была в основном состоянии?

а) Решите задачу в представлении взаимодействия. Обратите внимание, что матричные элементы возмущения отличны от нуля только между соседними уровнями. Следовательно, при малом E вероятность перехода в n - состояние дается n-м порядком теории возмущений. При каком соотношении между E, ω и τ теория возмущений работает?

б)* Для произвольных E и τ найдите точную S-матрицу и вероятность перехода из основного в n-е состояние.

Solution. в представлении взаимодействия и теорией возмущений

$$\hat{\mathcal{H}}_{\text{int}} = -eEe^{i\hat{\mathcal{H}}_0 t}\hat{x}^{-i\hat{\mathcal{H}}_0 t},$$

$$\langle m|\hat{\mathcal{H}}_{\text{int}}(t)|n\rangle = -eEe^{i(m-n)\omega t}\langle m|\hat{x}|n\rangle.$$

$$\langle m|\hat{x}|n\rangle := l_0\langle m|a + a^+|n\rangle = l_0\left(\delta_{m,n+1}\sqrt{m} + \delta_{m+1,n}\sqrt{n}\right),$$

$l_0 := \sqrt{h/2m\omega}$.

$$\langle m|\hat{\mathcal{H}}_{\text{int}}(t)|n\rangle = -eEl_0\left(\delta_{m,n+1}\sqrt{m}e^{i\omega t} + \delta_{m+1,n}\sqrt{n}e^{-i\omega t}\right).$$

Далее,

$$i\hbar\dot{\psi} = \hat{\mathcal{H}}_{\text{int}}\psi,$$

$$\psi(t) = \psi(0) - \frac{i}{\hbar}\int_0^t \hat{\mathcal{H}}_{\text{int}}(t')\,\psi(t')\,dt'.$$

Это уравнение говорит, $(n+1)$-я поправка к функции (за счет левой части) определяется функцией в n-ом порядке ТВ и оператором перехода в ближайшие состояния (за счет правой части). Таким образом, в каждом порядке появляется вероятность перехода на больший уровень. Другими словами, проекция $\langle n|\psi(t)\rangle$ отлична от нуля только начиная с n-го порядка теории возмущений:

$$\langle n|\psi^{(n)}(t)\rangle = -i\int_0^t \langle n|\hat{\mathcal{H}}_{\text{int}}(t')\,|\psi^{(n-1)}(t')\rangle dt' = \frac{ieEl_0}{\hbar}\sqrt{n}\int_0^t e^{i\omega t'}\langle n-1|\psi^{(n-1)}(t')\rangle dt',$$

где индекс (n) состояния $\psi^{(n)}(t)$ означает порядок теории возмущений.

$$u_n(t) = \langle n|\psi^{(n)}(t)\rangle, \qquad u_0(t) = 1$$

$$u_n(t) = \frac{ieEl_0}{\hbar}\sqrt{n}\int_0^t e^{i\omega t'}u_{n-1}(t')\,dt',$$

$$u_n(t) = \left(\frac{eEl_0}{\hbar\omega}\right)^n \frac{1}{\sqrt{n!}}\left(e^{i\omega t} - 1\right)^n.$$

$$W_{0\to n} = |u_n(\tau)|^2 = \left(\frac{e^2E^2}{2m\omega^3 h}\right)^n \frac{1}{n!}\left(2\sin\frac{\omega\tau}{2}\right)^{2n} = \frac{1}{n!}\left[\frac{e^2E^2(1-\cos\omega\tau)}{m\omega^3 h}\right]^n.$$

Теория возмущений работает, если $\frac{e^2E^2(1-\cos\omega\tau)}{m\omega^3 h} \ll 1$.

Точная вероятность перехода проекциями

$$\hat{\mathcal{H}} \equiv \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}}$$
$$\hat{\mathcal{H}}_0 = \hbar\omega\left(a^+a + 1/2\right), \quad \hat{\mathcal{H}}_{\text{int}} = -eE\hat{x} = -eEl_0\left(a + a^+\right),$$

$\left(l_0 = \sqrt{\hbar/2m\omega}\right)$.

Пусть $\hat{\mathcal{H}}_{\text{int}} = 0$:

$$\dot{a} = (i/\hbar)\left[\hat{\mathcal{H}}_0, a\right] = i\omega\left[a^+a, a\right] = -i\omega a, \qquad \dot{a}^+ = i\omega a^+.$$

$$a(t) = ae^{-i\omega t}, \qquad a^+(t) = a^+e^{i\omega t}.$$

Пусть $\hat{\mathcal{H}}_{\text{int}} \neq 0$:

$$\dot{a} = (i/h)\left[\hat{\mathcal{H}}_{\text{int}}, a\right] = ieEl_0e^{-i\omega t}.$$

$$a(\tau) = a(0) - iEl_0\int\limits_0^\tau e^{-i\omega t}dt = a(0) + \mu,$$

$$\mu := \frac{eEl_0}{\hbar\omega}\left(e^{-i\omega\tau} - 1\right)$$

$$|n, t = \tau\rangle = \frac{\left(a^+(\tau)\right)^n}{\sqrt{n!}}|0, t = \tau\rangle = \frac{\left(a^+(0) + \mu^*\right)^n}{\sqrt{n!}}|0, t = \tau\rangle.$$

$$\langle n, t = \tau|0, t = 0\rangle = \langle 0, t = \tau|\frac{(a(0) + \mu)^n}{\sqrt{n!}}|0; t = 0\rangle = \frac{\mu^n}{\sqrt{n!}}\langle 0, t = \tau|0, t = 0\rangle.$$

$$W_{0\to n} = \frac{|\mu|^{2n}}{n!}W_{0\to 0},$$

$$\sum_n W_{0\to n} = 1 \qquad \Rightarrow \qquad W_{0\to 0} = e^{-|\mu|^2}.$$

Получается распределение Пуассона

$$W_{0\to n} = \frac{|\mu|^{2n}}{n!}e^{-|\mu|^2} \qquad |\mu|^2 := e^2E^2/m\hbar\omega^3(1 - \cos\omega\tau)$$

При малых μ ответ совпадает с результатом, полученным по теории возмущений, как и должно быть.

Точная S-матрица переходом к когерентным состояниям (???)

Приведем решение, показывающее связь задачи с когерентными состояниями осциллятора, определяемыми как собственные состояния оператора уничтожения a.

$$\hat{\mathcal{H}} = \hbar\omega\left[a^+a + \frac{1}{2} + \lambda\left(a^+ + a\right)\right], \qquad \lambda := -eEl_0/\hbar\omega$$
$$b := a + \lambda, \qquad b^+ := a^+ + \lambda.$$

Поскольку $[b, b^+] = 1$, переход от a и a^+к b и b^+ определяет каноническое преобразование, при этом гамильтониан становится чисто осцилляторным:

$$\hat{\mathcal{H}} = \hbar\omega\left(b^+b + \frac{1}{2} - \lambda^2\right).$$

Введем собственные состояния оператора уничтожения b:

$$b|\eta\rangle = \eta|\eta\rangle.$$

Здесь η может быть любым комплексным числом. Нетрудно проверить, что

$$|\eta\rangle = e^{-|\eta|^2/2}\sum_{n=0}^{\infty}\frac{\eta^n}{\sqrt{n!}}|n\rangle,$$

где $|n\rangle$ - состояния полученного гамильтониана, отвечающие энергии $E_n = h\omega\left(n + 1/2 - \lambda^2\right)$. Возьмем состояние осцилллтора до включения поля: $a|0_a\rangle = 0$. Используя связь a и b, находим

$$b|0_a\rangle = \lambda|0_a\rangle,$$

$$|0_a\rangle = e^{-\lambda^2/2}\sum_{n=0}^{\infty}\frac{\lambda^n}{\sqrt{n!}}|n_b\rangle.$$

Разложение по состояниям $|n_b\rangle$ позволяет сразу написать зависимость от времени:

$$|0_a\rangle(t) = \exp\left(-\frac{i}{\hbar}\hat{\mathcal{H}}t\right)|0_a\rangle = e^{i\left(\lambda^2-1/2\right)\omega t}e^{-\lambda^2/2}\sum_{n=0}^{\infty}\frac{\left(\lambda e^{-i\omega t}\right)^n}{\sqrt{n!}}|n_b\rangle,$$

т.е.

$$b|0_a\rangle(t) = \lambda e^{-i\omega t}|0_a\rangle(t),$$
$$a|0_a\rangle(t) = \lambda\left(e^{-i\omega t} - 1\right)|0_a\rangle(t).$$

Обозначив $\mu = \lambda\left(e^{-i\omega t} - 1\right)$, получаем

$$|0_a\rangle(t) = S(t)|0_a\rangle = e^{-|\mu|^2/2}\sum_{n=0}^{\infty}\frac{\mu^n}{\sqrt{n!}}|n_a\rangle.$$

Отсюда находим столбец S-матрицы: $\langle n|\hat{S}(t)|0\rangle = e^{-|\mu|^2/2}\mu^n/\sqrt{n!}$. Искомые вероятности переходов есть

$$W_{0\to n} = e^{-|\mu|^2}\frac{|\mu|^{2n}}{n!} = \frac{1}{n!}\left[\frac{e^2E^2(1-\cos\omega t)}{m\omega^3\hbar}\right]^n\exp\left[-\frac{e^2E^2(1-\cos\omega t)}{m\omega^3\hbar}\right]$$

Остальные матричные элементы можно получить из соотношений для зависящих от времени операторов: $\hat{S}b^+ = b^+\hat{S}e^{-i\omega t}, \hat{S}a^+ = a^+\hat{S}e^{-i\omega t} + \mu\hat{S}$. Отсюда

$$\langle n|\hat{S}|k\rangle = \frac{1}{\sqrt{k}}\langle n|\hat{S}a^+|k-1\rangle = \frac{1}{\sqrt{k}}\langle n|a^+\hat{S}e^{-i\omega t} + \mu\hat{S}|k-1\rangle$$

и получается рекуррентная формула:

$$\langle n|\hat{S}|k\rangle = \frac{\sqrt{n}}{\sqrt{k}}e^{-i\omega t}\langle n-1|\hat{S}|k-1\rangle - \frac{\mu}{k}\langle n|\hat{S}|k-1\rangle.$$

Применяя её достаточно много раз, выражаем $\langle n|\hat{S}|k\rangle$ через $\langle 0|\hat{S}|0\rangle = e^{-|\mu|^2/2}$:

$$\langle n|\hat{S}|m\rangle = \frac{e^{-|\mu|^2/2}}{\sqrt{m!n!}}\sum_{k=0}^{\min(m,n)}\frac{n!m!}{k!(n-k)!(m-k)!}\mu^{n+m-2k}e^{-i\omega kt}.$$

ФР.? Линейное появление поля

Для заряженного линейного гармонического осциллятора, находящегося первоначально в основном состоянии, определить вероятности переходов в различные возбужденные состояния под влиянием однородного электрического поля вида

$$\mathcal{E} = \begin{cases} 0, & t < 0, \\ \mathcal{E}_0\frac{t}{\tau}, & 0 \leqslant t \leqslant \tau, \\ \mathcal{E}_0, & t > \tau \end{cases}$$

Solution.

$$\hat{\mathrm{H}} = \frac{\hat{\mathrm{p}}^2}{2m} + \frac{m\omega^2x^2}{2} - e\varepsilon x,$$

последнее слагаемое учтем по теории возмущений.

$$V_{10} = -e\mathcal{E}\langle 1|\hat{x}|0\rangle = -\frac{e\mathcal{E}x_0}{\sqrt{2}}, \quad x_0 = \sqrt{\frac{\hbar}{m\omega}},$$

остальные в 1 порядке нулевые.

$$a_{0n}^{(1)} = \frac{1}{i\hbar}\int\limits_{-\infty}^{+\infty} V_{n0}\left(t'\right) e^{i\omega_{n0}t'}dt' = -\frac{1}{i\hbar}\int\limits_{-\infty}^{+\infty} \mathcal{E}_0\frac{t}{\tau}\frac{ex_0}{\sqrt{2}}e^{i\omega_{n0}t'}dt'$$

Проинтегрируем по частям и отбросим внеинтегральное слагаемое, считая, что оно не вносит вклада в квантовые переходы (??????????????):

$$a_{0n}^{(1)} = -i\int\limits_0^{\tau} \frac{e}{\sqrt{2}}\sqrt{\frac{\hbar}{m\omega}}\frac{\mathcal{E}_0}{\tau}\frac{e^{i\omega_{n0}t'}}{\hbar\omega_{n0}}dt' = \frac{e\mathcal{E}_0}{\sqrt{2\hbar m\omega}\omega\tau}\cdot 2e^{i\omega\tau/2}\sin(\omega\tau/2),$$

since $\mathrm{sh}(ix) = i\sin x$.

$$W_{0\to 1} = W_0\frac{\sin^2\left(\frac{\omega\tau}{2}\right)}{\left(\frac{\omega\tau}{2}\right)^2}, \qquad W_0 = \frac{e^2\mathcal{E}_0^2}{2\hbar m\omega}.$$

В случае мгновенного включения поля ($\omega\tau \ll 1$) имеем $W_{0\to 1} \simeq W_0$. При адиабатически медленном включении поля ($\omega\tau \gg 1$) получим $W_{0\to 1} \simeq 0$, т. е. переходы в возбужденные состояния практически не происходят. Это и ожидаемо.

Теория возмущений применима, если $V_{10} \ll \Delta E_{10}$, т.е.:

$$\frac{e\mathcal{E}_0}{\sqrt{2}}\sqrt{\frac{\hbar}{m\omega}} \ll \hbar\omega$$

17.2.8 Problems about central field 1

Б-2.6.1

Записать уравнение Шредингера для двух частиц с массами m_1 и m_2, взаимодействующих по закону $U\left(\mathbf{r}_1 - \mathbf{r}_2\right)$ в системе центра масс. Какой вид имеет волновая функция $\Psi\left(\mathbf{r}_1, \mathbf{r}_2\right)$?

Solution.

2.6.1. Система двух частиц описывается волновой функцией $\Psi\left(\mathbf{r}_1, \mathbf{r}_2, t\right)$, которая подчиняется уравнению Шредингера

$$i\hbar\frac{\partial}{\partial t}\Psi\left(\mathbf{r}_1, \mathbf{r}_2, t\right) = \hat{\mathrm{H}}\Psi\left(\mathbf{r}_1, \mathbf{r}_2, t\right),$$

причем гамильтониан в координатном представлении имеет вид

$$\hat{\mathrm{H}} = -\frac{\hbar^2}{2m_1}\Delta_1 - \frac{\hbar^2}{2m_2}\Delta_2 + U\left(\mathbf{r}_1 - \mathbf{r}_2\right).$$

Введем координату центра масс $\mathbf{R}$ и относительную координату $\mathbf{r}$:

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2.$$

Проделав далее замену переменных $\mathbf{r}_1, \mathbf{r}_2, \Delta_1, \Delta_2 \to \mathbf{R}, \mathrm{r}, \Delta_{\mathbf{R}}, \Delta_{\mathrm{r}}$ (используя правило дифференцирования сложной функции), приведем гамильтониан к виду

$$\hat{\mathrm{H}} = -\frac{\hbar^2}{2M}\Delta_{\mathbf{R}} - \frac{\hbar^2}{2\mu}\Delta_{\mathbf{r}} + U(\mathbf{r}),$$

где $M = m_1 + m_2, \mu = m_1m_2/M$ - соответственно полная и приведенная массы. Ввиду того, что система стационарна, полагаем, что волновая функция будет иметь вид

$$\Psi\left(\mathbf{r}_1, \mathbf{r}_2, t\right) = e^{-\frac{1}{\hbar}Et}\Phi(\mathbf{R})\psi(\mathbf{r}), \quad E = E_{\text{цм}} + E_{\text{отн.}}\ .$$

Полная энергия складывается из энергии движения центра масс $E_{\text{им и}}$ энергии относительного движения $E_{\text{отн.}}$. Функции $\Phi(\mathbf{R})$ и $\psi(\mathbf{r})$ должны подчиняться уравнениям

$$-\frac{\hbar^2}{2M}\Delta_{\mathbf{R}}\Phi(\mathbf{R}) = E_{\text{цМ}}\ \Phi(\mathbf{R}),$$
$$\left[-\frac{\hbar^2}{2\mu}\Delta_{\mathbf{r}} + U(\mathbf{r})\right]\psi(\mathbf{r}) = E_{\text{отн}}\ \psi(\mathbf{r}).$$

Из уравнения (1) следует, что функция $\Phi(\mathbf{R})$ описывает свободное движение центра масс: $\Phi(\mathbf{R}) = Ce^{\frac{i}{\hbar}\text{PR}}$, характеризуемое полным импульсом $\mathbf{P}$ и энергией $E_{\text{шм}} = \mathbf{P}^2/(2M)$.

Б-2.6.2

Определить интегралы движения для частицы, движущейся в произвольном центральном поле.

Solution.

2.6.2. Операторы $\hat{1}^2, \hat{i}_x, \hat{I}_y, \hat{I}_z, \hat{I}$ коммутируют с гамильтонианом и являются интегралами движения в произвольном центральном поле.

Б-2.6.3

Найти волновую функцию основного состояния атома водорода в импульсном представлении.

Solution.

2.6.3. Используя явный вид волновой функции основного состояния водородоподобного атома в координатном представлении

$$\psi_{100}(\mathbf{r}) = \frac{Z^{3/2}}{\sqrt{\pi}}e^{-Zr},$$

перейдем в импульсное представление:

$$\phi(\mathbf{p}) = \frac{1}{(2\pi)^{3/2}}\int d^3x e^{-i(\mathbf{rp})}\psi_{100}(\mathbf{r}) = \frac{\sqrt{8Z^5}}{\pi}\frac{1}{\left(Z^2+p^2\right)^2}.$$

Б-2.6.4 Средние и теорема вириала в водороде

Найти среднее значение операторов $r^2, 1/r, \hat{\mathbf{p}}^2$ для основного состояния атома водорода. Убедиться в том, что выполняется теорема вириала.

Solution.

2.6.4. Приводим ответы: $\langle r^2\rangle = 3/Z, \langle 1/r\rangle = Z, \langle\hat{\mathbf{p}}^2\rangle = Z^2$. Учитывая, что средняя кинетическая энергия $\langle\hat{\text{T}}\rangle = \langle\hat{\mathbf{p}}^2/2\rangle$, а средняя потенциальная энергия $\langle\hat{\text{U}}\rangle = -\langle Z/r\rangle$, убеждаемся в справедливости теоремы вириала для кулоновских сил:

$$2\langle\hat{\text{T}}\rangle + \langle\hat{\text{U}}\rangle = 0.$$

Б-2.6.5 Средние $\langle 1/r\rangle$ и $\langle 1/r^2\rangle$ в водороде

С помощью теоремы Фейнмана-Гельмана получить $\langle 1/r\rangle$ и $\langle 1/r^2\rangle$ в произвольном состоянии атома водорода. Используя теорему Эренфеста для радиального движения $d\langle\hat{\text{p}}_r\rangle/dt = \langle\hat{\text{F}}_r\rangle$, получить $\langle 1/r^3\rangle$ для состояний атома водорода $cl > 0$.

Solution.

$$\begin{cases} \hat{\mathrm{H}} = \frac{\hat{\mathrm{p}}_r}{2} + \frac{l(l+1)}{2r^2} - \frac{Z}{r}. \\ \varepsilon_n = -\frac{Z^2}{2n^2}. \end{cases}$$

Учитывая теорему Фейнмана-Гельмана (задача 2.1.22), а также очевидные соотношения

$$\frac{\partial \hat{\mathrm{H}}}{\partial Z} = -\frac{1}{r}, \quad \frac{\partial \varepsilon_n}{\partial Z} = -\frac{Z}{n^2}, \quad \text{получаем} \quad \langle \frac{1}{r} \rangle = \frac{Z}{n^2},$$

где угловыми скобками обозначено среднее по произвольному состоянию атома водорода $|n|m\rangle$. Имея в виду далее, что

$$\frac{\partial \hat{\mathrm{H}}}{\partial l} = \frac{l+1/2}{r^2}, \quad \frac{\partial \varepsilon_n}{\partial n} = \frac{Z^2}{n^3}, \quad \text{получаем} \quad \langle \frac{1}{r^2} \rangle = \frac{Z^2}{n^3(l+1/2)}$$

Здесь мы использовали связь квантовых чисел $n = n_r + l + 1$ для атома водорода. При дифференцировании выражений, например, по l, мы считали зависимость от l непрерывной, т. е. вместо реальной дискретной переменной l мы рассматривали некоторую фиктивную непрерывную переменную, равную / в точках, отвечающих целым значениям $l = 0, 1, ...$ Из теоремы Эренфеста для радиального движения

$$\frac{d\langle \hat{\mathrm{p}}_r \rangle}{dt} = \langle \hat{\mathrm{F}}_r \rangle = -\langle \frac{\partial \hat{\mathrm{H}}}{\partial r} \rangle = \frac{i}{\hbar} \langle \left[\hat{\mathrm{H}}, \hat{\mathrm{p}}_r \right] \rangle$$

легко получить, что

$$\langle \hat{\mathrm{H}} \hat{\mathrm{p}}_r - \hat{\mathrm{p}}_r \hat{\mathrm{H}} \rangle = 0, \quad \text{откуда } \langle \frac{\partial \hat{\mathrm{H}}}{\partial \mathrm{r}} \rangle = 0.$$

На основании этого окончательно находим

$$\langle \frac{1}{r^3} \rangle = \frac{Z^3}{n^2(l+1/2)l(l+1)}, \quad l > 0.$$

Б-2.6.6

Записать стационарное уравнение Шредингера для атома водорода в импульсном представлении.

Solution.

Записать-то запросто, а вот про решение много можно думать, но тут не спрашивается эт.

$$\left(\frac{\mathbf{p}^2}{2} - E \right) \phi(\mathbf{p}) = -\int d^3p' W(\mathbf{p} - \mathbf{p}') \phi(\mathbf{p}')$$

$$W(\mathbf{p}) = \frac{1}{(2\pi)^3} \int d^3x e^{-i(\mathbf{r})} U(\mathbf{r})$$

Для $U(r) = -\frac{Z}{r}$ нетрудно получить $W(p) = -\frac{Z}{2\pi^2 p^2}$, и уравнение примет вид

$$\left(p^2 - 2E \right) \phi(\mathbf{p}) = \frac{Z}{\pi^2} \int d^3p' \frac{\phi(\mathbf{p})}{|\mathbf{p} - \mathbf{p}'|^2}$$

Полученное уравнение можно свести к одномерному интегральному уравнению, точное решение которого впервые было найдено В. А. Фоком (1935 г.). (??? потом изучу)

17.2.9 Problems about central field 2

Б-2.6.7 Решение осциллятора в ДСК и СфСК

Найти уровни энергии трехмерного изотропного осциллятора и кратности их вырождения, разделяя переменные:
а) в декартовых координатах;
б) в сферических координатах.
Определить четность состояний. Обсудить связь задачи с моделью ядерных оболочек и получить первые три магических числа: 2, 8, 20.

Solution. а), в ДСК

$$\left\{-\frac{\hbar^2}{2m}\Delta+\frac{m\omega^2\mathbf{r}^2}{2}\right\}\psi(\mathbf{r})=E\psi(\mathbf{r}).$$

$$\hat{\mathrm{H}}=\sum_{i=1}^{3}\left\{-\frac{h^2}{2m}\frac{\partial^2}{\partial x_i^2}+\frac{m\omega^2x_i^2}{2}\right\}.$$

где $x_i=x,y,z$, то очевидно, что решение может быть представлено в виде

$$\psi_{n_1n_2n_3}(\mathbf{r})=u_{n_1}^{\mathrm{ocu}}\,(x)u_{n_2}^{\mathrm{ocul}}\,(y)u_{n_3}^{\mathrm{ocu}}\,(z),\quad n_1,n_2,n_3=0,1,2,...,$$
$$E_n=h\omega\left(n+\frac{3}{2}\right),\quad n=n_1+n_2+n_3,\quad n=0,1,2,...,$$

где $u_{n_i}^{\mathrm{осц}}\,(x_i)$ - собственные функции гамильтониана одномерного осциллятора (II.18):

$$u_{n_i}^{\mathrm{ocu}}\,(x_i)=\frac{1}{\sqrt{2^{n_i}n_i!x_0\sqrt{\pi}}}e^{-\frac{1}{2}\left(\frac{x_i}{x_0}\right)^2}H_{n_i}\left(\frac{x_i}{x_0}\right).$$

Здесь $H_{n_i}\,(x_i)$ - полиномы Эрмита, $x_0=\sqrt{\hbar/(m\omega)}$ - осцилляторная единица длины (II.16). Поскольку четность полиномов Эрмита $H_{n_i}\,(x_i)$ равна $I_{n_i}=(-1)^{n_i}$, то состояния (2) и уровни энергии (3) также характеризуются определенной четностью

$$I_n=(-1)^{n_1+n_2+n_3}=(-1)^n.$$

При вычислении кратности вырождения уровней энергии (3) заметим, что, если задать n_1, то число n_2 будет принимать значения $n_2=0,1,...,n-n_1$, т. е. всего $n-n_1+1$ различных значений. Число n_3 всегда фиксировано соотношением $n_3=n-n_1-n_2$. Поэтому полная кратность вырождения уровня энергии будет равна

$$\sum_{n_1=0}^{n}(n-n_1+1)=\frac{1}{2}(n+1)(n+2).$$

Solution. а), в сферических координатах

(!!!???????!!! впишу про это в 1ю часть!!!)

$$\left\{-\frac{\hbar^2}{2m}\Delta+\frac{m\omega^2\mathbf{r}^2}{2}\right\}\psi(\mathbf{r})=E\psi(\mathbf{r}).$$

$$\psi_{Elm}(\mathbf{r})=R_{El}(r)Y_l^{(m)}(\theta,\varphi),$$

где $Y_l^{(m)}(\theta,\varphi)$ - сферическая функция, а функция $R_{EL}(r)$ должна удовлетворять уравнению

$$R''(r)+\frac{2}{r}R'(r)+\left\{\frac{2mE}{\hbar^2}-\frac{r^2}{r_0^4}-\frac{l(l+1)}{r^2}\right\}R(r)=0.$$

где $r_0=\sqrt{\hbar/(m\omega)}$ - осцилляторная единица длины (II.16). Переходя в уравнении (4) к безразмерным переменным, получим

$$R''(q)+\frac{2}{q}R'(q)+\left\{2\varepsilon-q^2-\frac{l(l+1)}{q^2}\right\}R(q)=0,$$

где $q=r/r_0,\varepsilon=E/(\hbar\omega)$. Исследуем асимптотики функции $R(q)$. При $q\to 0$ имеем следующий асимптотический вид уравнения (5):

$$R_0''+\frac{2}{q}R_0'-\frac{l(l+l)}{q^2}R_0=0.$$

Ищем решение этого уравнения, как обычно, в виде $R_0\sim q^5$ и получаем для s уравнение и его решения в виде

$$s(s-1)+2s-l(l+1)=0,\quad\to s_1=l,\quad s_2=-(l+1).$$

Следовательно, асимптотика радиальной функции при $q \to 0$ имеет вид $R|_{q\to 0} \sim q^l$, поэтому сделаем подстановку $R(q) = q^l u(q)$. Для функции $u(q)$ получим уравнение

$$u'' + \frac{2(l+1)}{q}u' + \left(2\varepsilon - q^2\right)u = 0.$$

Асимптотику функции $u(q)$ при $q \to \infty$ определим из уравнения Подставляя в данное уравнение $u_\infty \sim e^{-\alpha q^2}$, находим $\alpha = 1/2$. Таким образом, радиальную функцию с выделенными асимптотиками можно записать в виде

$$R(q) = e^{-q^2/2} q^l w(q),$$

учитывающем особенности поведения в нуле и на бесконечности. Введем новую переменную согласно $\xi = q^2$, и получим уравнение для функции $w(\xi)$:

$$\xi \frac{d^2 w}{d\xi^2} + \left\{\left(l + \frac{3}{2}\right) - \xi\right\}\frac{dw}{d\xi} - \left\{\frac{1}{2}\left(l + \frac{3}{2}\right) - \frac{\varepsilon}{2}\right\} w = 0.$$

Функцию $w(\xi)$ мы будем далее искать в виде суммы степенного ряда

$$w(\xi) = \sum_{k=0}^{\infty} a_k \xi^k.$$

Подставляя в (7) решение в виде суммы (8) и, группируя члены с одинаковыми степенями ξ, находим

$$\sum_{k=0}^{\infty} \xi^k \left[(k+1)\left(k + l + \frac{3}{2}\right) a_{k+1} - \left(\frac{1}{2}\left(l - \varepsilon + \frac{3}{2}\right) - k\right) a_k\right] = 0.$$

Отсюда, приравнивая нулю коэффициенты при ξ^k, найдем рекуррентные соотношения для коэффициентов a_k:

$$a_{k+1} = a_k \frac{(l + 3/2 - \varepsilon) + 2k}{(k+1)(2(k+l)+3)}.$$

Поскольку в ряде (8) отношение двух последующих коэффициентов в соответствии с (9) при $k \gg 1$ стремится к пределу

$$\left.\frac{a_{k+1}}{a_k}\right|_{k\gg 1} \to \frac{1}{k},$$

то при больших значениях аргумента, т. е. при $\xi \to \infty$ мы получим $w(\xi) \sim e^{\xi}$ или $w(q) \sim e^{q^2}$ (см. Б-2.5.2). Поэтому радиальная функция (6) при $q \to \infty$ будет экспоненциально расти: $R(q)|_{q\to\infty} \sim e^{q^2/2}$. Чтобы избежать данного неограниченного роста, необходимо «оборвать» ряд (8) при некотором $k = n_r$, т. е. свести его к полиному. При этом должно выполняться условие

$$\frac{1}{2}\left(l + \frac{3}{2} - \varepsilon\right) = -n_r, \quad n_r = 0, 1, 2, ...,$$

откуда получаем уровни энергии:

$$E_n = \hbar\omega\left(l + 2n_r + \frac{3}{2}\right) = \hbar\omega\left(n + \frac{3}{2}\right), \quad n = 2n_r + l = 0, 1, 2, ...$$

Здесь n_r - радиальное, l - орбитальное и n - главное квантовое число,

Для функции $w(\xi)$ мы имеем ряд (8), который определяется рекуррентными соотношениями (9) и сводится к вырожденной гипергеометрической функции $F(-n_r, l + 3/2, \xi)$, которая является регулярным при $\xi \to 0$ решением [4)] уравнения (7). При условии (10) гипергеометрическая функция превращается в присоединенный полином Лагерра (см. (Д.24)), т. е.

$$w_{n_r l}(\xi) = a_0\left[1 - \frac{n_r}{(l+3/2)}\frac{\xi}{l} + \frac{n_r(n_r-1)}{(l+3/2)(l+3/2+1)}\frac{\xi^2}{2} + ...\right] =$$
$$= a_0 F(-n_r, l+3/2, \xi) = \frac{a_0\Gamma(l+3/2)}{\Gamma(l+3/2+n_r)} L_{n_r}^{l+1/2}(\xi).$$

Здесь константа a_0 определяется из условия нормировки. Восстанавливая исходные обозначения, запишем общий вид радиальной функции $R(r)$, нормированной условием $\int\limits_0^\infty |R(r)|^2 r^2 dr = 1$:

$$R_{n_r l}(r) = \sqrt{\frac{2}{r_0^3 n_r! \Gamma\left(l+3/2+n_r\right)}} e^{-\frac{1}{2}\left(\frac{r}{r_0}\right)^2} \left(\frac{r}{r_0}\right)^l L_{n_r}^{l+\frac{1}{2}}\left(\left(\frac{r}{r_0}\right)^2\right).$$

Таким образом, полная волновая функция в сферической системе координат

$$\psi_{nlm}(\mathbf{r}) = R_{nl}(r) Y_l^{(m)}(\theta, \varphi)$$

зависит от трех квантовых чисел: n, l и m (функцию (11) можно записать с учетом $n_r = (n-l)/2$), в то время, как уровни энергии определяются только главным квантовым числом n. Поэтому имеется вырождение: уровню энергии с определенным значением числа n отвечают функции с $l = n, n-2, ...0$, если n - четное ($n/2+1$ значений l), или с $l = n, n-2, ..., l$, если n - нечетное ($(n+1)/2$ значений l). Кроме того, для каждого / существует $2l+1$ различных значений магнитного квантового числа m (уровни энергии не зависят от m).

На основании этого заключаем, что уровни энергии имеют определенную четность [5)] $I_n = (-1)^n = (-1)^l$ и полную кратность вырождения (для четного и нечетного n), равную

$$\sum_{l=0,2,...}^{n} (2l+1) = \sum_{l=1,3,...}^{n} (2l+1) = \frac{1}{2}(n+1)(n+2).$$

что полностью соответствует результату п. а). Потенциал изотропного гармонического осциллятора можно использовать в качестве модели самосогласованного поля, которое действует на каждый нуклон в ядре (модель ядерных оболочек). При этом найденные нами уровни энергии (3) представляют собой спектр одночастичных уровней для рассматриваемой модели. Если главное квантовое число принимает значения $n = 0, 1, 3$, то максимальное число нуклонов, которые могут находиться на соответствующих уровнях равно $2, 6, 12$ (удвоение кратности вырождения (12) связано с тем, что нуклоны имеют спин $1/2$). Максимальное число нуклонов, которые можно разместить на всех уровнях, начиная с нулевого и заканчивая рассматриваемым, будет равно $2, 8, 20$. Это и есть значения магических чисел для данной модели оболочек.

Б-2.6.8 Трехмерный колодец

Найти уровни энергии и волновые функции частицы в трехмерном потенциальном ящике:

$$U(x) = \begin{cases} 0, & r < a \\ \infty, & r \geqslant a \end{cases}$$

Сравнить порядок следования уровней энергии в этой задаче и трехмерного изотропного осциллятора.

Solution.

2.6.8. Уравнение Шредингера для данного потенциала допускает разделение переменных в сферической системе координат, и его решение можно представить в виде (см. (II.33))

$$\psi(\mathbf{r}) = R_l(r) Y_l^{(m)}(\theta, \varphi) = \frac{1}{r} \chi_l(r) Y_l^{(m)}(\theta, \varphi).$$

В результате такой подстановки мы получаем для функции $\chi_l(r)$ так называемое «укороченное» радиальное уравнение

$$\chi_l''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right)\chi_l(r) = 0, \qquad \text{где} \qquad E = \frac{\hbar^2 k^2}{2m}.$$

Функция χ_l удовлетворяет данному уравнению при $0 < r < a$, и должна быть равна нулю при $r = 0$ и при $r \geqslant a$.

Случай $l = 0$.

В этом случае УШ и граничные условия $\chi_l(0) = \chi_l(a) = 0$ имеют точно такой же вид, как и в одномерной задаче (см. задачу 2.2.1). На основании этого сразу получаем решение:

$$E_{n_r 0} = \frac{\pi^2 \hbar^2}{2ma^2} n_r^2, \qquad \psi_{n_r 0} = \begin{cases} \frac{1}{\sqrt{2\pi a r}} \sin \frac{\pi n_r}{a} r, & 0 < r < a \\ 0, & r \geqslant a \end{cases}$$

где $n_r = 1, 2, 3, ...$ - радиальное квантовое число.

Случай $l > 0$.

При помощи замены $\chi_l(r) = \sqrt{r}\varphi(r)$ УШ приводится к виду

$$\varphi'' + \frac{1}{r}\varphi' + \left[k^2 - \frac{(l+1/2)^2}{r^2}\right]\varphi = 0.$$

Решениями данного уравнения являются функции Бесселя полуцелого порядка $J_{\pm(l+1/2)}(kr)$. Поэтому общее решение УШ можно записать в виде

$$\chi_l(r) = C_1 j_l(kr) + C_2 n_l(kr),$$

$$j_l(x) := \sqrt{\frac{\pi x}{2}} J_{l+1/2}(x)$$

$$n_l(x) := \sqrt{\frac{\pi x}{2}} N_{l+1/2}(x) = (-1)^{l+1}\sqrt{\frac{\pi x}{2}} J_{-(l+1/2)}(x).$$

$$j_l(x)|_{x\to 0} \simeq \frac{x^{l+1}}{(2l+1)!!}, \quad n_l(x)|_{x\to 0} \simeq -\frac{(2l-1)!!}{x^l}.$$

Из граничного условия $\chi_l(0) = 0$ и асимптотики следует, что решение УШ необходимо выбрать в виде

$$\chi_l(r) = c j_l(kr).$$

Граничное условие $\chi_l(a) = 0$ определяет значения k и, следовательно, - уровни энергии и собственные функции. Должно выполняться условие

$$j_l(ka) = 0, \quad \text{или} \quad J_{l+1/2}(ka) = 0,$$

поэтому окончательно находим

$$E_{n_r l} = \frac{\pi^2 h^2}{2ma^2}\lambda^2_{n_r l}, \qquad R_{n_r l}(r) = \begin{cases} \frac{c}{r} j_l\left(\frac{\lambda_{n_r l}}{a} r\right), & 0 < r < a, \\ 0, & r \geqslant a, \end{cases}$$

где $\lambda_{n,l}$ - корни функции Бесселя $J_{l+1/2}(x), n_r = 1, 2, \ldots$ - радиальное квантовое число, определяющее номер корня в порядке возрастания его величины. Вырождение по орбитальному квантовому числу отсутствует значение энергии однозначно определяет число l. Вырождение по магнитному квантовому числу m существует, ибо оно обусловлено сферической симметрией задачи.

Используя значения корней $\lambda_{n_r l}$, можно определить порядок расположения уровней энергии, начиная от основного состояния: $1s, 1p, 1d, 2s, 1f, 2p, 1g, 2d, 1h, 3s, 2f, \ldots$, где состояния с $l = 1, 2, 3, 4, 5, \ldots$ обозначаются буквами $s, p, d, f, g, h, \ldots$, число перед буквой нумерует уровни с одинаковым l в порядке возрастания их значений (очевидно, в данном случае это число просто равно n_r). Для сравнения приведем порядок расположения уровней для изотропного пространственного осциллятора (см. задачу 2.6.7, число перед буквой теперь равно $n + 1$) $1s, 1p, [1d, 2s], [1f, 2p], [1g, 2d, 3s], \ldots$. Для уровней энергии осциллятора характерно вырождение по квантовому числу l, поэтому состояния, отвечающие одному и тому же уровню, заключены в скобки. Заметим, что отличия в порядке расположения начинают проявляться лишь для сравнительно высоко лежащих уровней энергии.

Б-2.6.9 Трехмерная яма

Найти уровни энергии состояния частицы в трехмерной потенциальной яме вида

$$U(r) = \begin{cases} -U_0, & r < a, \\ 0, & r \geqslant a. \end{cases}$$

Solution.

Как и в предыдущей задаче, представим решение уравнения Шредингера в виде

$$\psi(\mathbf{r}) = R_l(r) Y_l^{(m)}(\theta, \varphi) = \frac{1}{r}\chi_l(r) Y_l^{(m)}(\theta, \varphi).$$

$$\varkappa^2 := \frac{2m}{\hbar^2}|E|, \qquad k^2 := k_0^2 - \varkappa^2, \qquad k_0^2 := \frac{2mU_0}{\hbar^2},$$

$$\chi_l''(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right)\chi_l(r) = 0 \qquad 0 < r < a,$$
$$\chi_l''(r) + \left(-\varkappa^2 - \frac{l(l+1)}{r^2}\right)\chi_l(r) = 0 \qquad r \geqslant a$$

Решение уравнения (1а), удовлетворяющее граничному условию $\chi_l(0) = 0$, представляет собой сферическую функцию Бесселя $\chi_l(r) = Aj_l(kr)$ при $0 < r < a$. Решением уравнения (1б), экспоненциально убывающим при $r \to \infty$, является сферическая функция Ханкеля мнимого аргумента (см. (Д.17)):

$$\chi_l(r) = Bh_l^{(1)}(i\varkappa r) \quad \text{при } r \geqslant a,$$
$$h_l^{(1)}(x) = j_l(x) + in_l(x).$$

Из условия непрерывности логарифмической производной на границе ямы $r = a$ получим

$$k\frac{j_l'(ka)}{j_1(ka)} = i\varkappa\frac{h_l^{(1)\prime}(i\varkappa a)}{h_l^{(1)}(i\varkappa a)}.$$

Очевидно, что это и есть трансцендентное уравнение, определяющеде уровни энергии связанных состояний в яме.

Для s-состояний ($l = 0$) уравнение (2) приобретает совсем простой вид:

$$k \operatorname{ctg} ka = -\varkappa.$$

Данное уравнение фактически совпадает с уравнением, определяющим уровни энергии для нечетных состояний задачи 2.2.2 (см. также задачу 2.2.4). Обсуждение вопросов о суцществовании связанных состояний и о количестве уровней энергии можно повторить здесь без особых изменений.

Б-2.6.10 Мелкая 2D яма

Найти энергию связанного состояния частицы в мелкой двумерной потенциальной яме. Сравнить с результатом для трехмерной потенциальной ямы.

Solution.

Уравнение Шредингера в импульсном представлении для двумерной потенциальной ямы имеет вид (см. задачу 2.6.6)

$$\left(\frac{\mathbf{p}^2}{2m} - E\right)\phi(\mathbf{p}) = -\int d^2p' W\left(\mathbf{p} - \mathbf{p}'\right)\phi\left(\mathbf{p}'\right) = -\int d^2q W(\mathbf{q})\phi(\mathbf{p} - \mathbf{q}),$$

$$\mathbf{q} := \mathbf{p} - \mathbf{p}',$$
$$W(\mathbf{q}) := \frac{1}{(2\pi\hbar)^2}\int d^2x e^{-i\frac{\mathbf{qr}}{\hbar}}U(\mathbf{r})$$

- фурье-образ потенциала взаимодействия. Полагаем, что потенциал обладает аксиальной симметрией $U(\mathbf{r}) = U(|\mathbf{r}|) = U(r)$, поэтому для фурье-образа будет также $W(\mathbf{q}) = W(q)$.

Не конкретизируя вид потенциала, предположим, что он имеет минимум, равный $-U_0$ и радиус действия a (т. е. при $r < a$ потенциал отличен от нуля). Тогда из очевидных свойств преобразования Фурье следует, что область локализации фурье-образа $W(q)$ в импульсном пространстве ограничена значением $q \lesssim \hbar/a$.

$$W(0) \simeq -\frac{U_0}{(2\pi\hbar)^2}\pi a^2$$

Далее мы полагаем, что яма мелкая, и координатная волновая функция связанного состояния при больших значениях r имеет вид убывающей экспоненты $\psi(r) \sim e^{-\varkappa r}$, причем выполняется условие $\kappa a \ll 1$ (см. также задачу 2.2.5). Поэтому область локализации функции в импульсном представлении, т. е. $\phi(q)$, должна быть $\sim \hbar\varkappa \ll \hbar/a$. Таким образом, при $q \to \infty$ функция $\phi(q)$ убывает значительно быстрее, чем $W(q)$. При этом доминирующую роль в интеграле (1) играет область $|q| \lesssim \hbar/a$, поэтому мы можем вынести $W(q)$ из-под знака интеграла в точке $q \approx 0$. В результате получим

$$\left(\frac{p^2}{2m} - E\right)\phi(p) = -W(0)\int d^2p\phi(p)$$

$$C := \int d^2p\phi(p)$$

$$\phi(p) = -\frac{2mCW(0)}{p^2 + 2m|E|}.$$

$$\left(\frac{p^2}{2m} - E\right)\left(-\frac{2mCW(0)}{p^2 + 2m|E|}\right) = -W(0)\int d^2p\left(-\frac{2mCW(0)}{p^2 + 2m|E|}\right)$$

$$1 = -W(0)\int\limits_0^\infty \frac{2m \cdot 2\pi p dp}{p^2 + 2m|E|} \simeq -W(0)2\pi m \ln\left(\frac{p^2}{2m} + |E|\right)\Big|_0^{\hbar/a}.$$

$W(0) \simeq -\frac{U_0}{(2\pi\hbar)^2}\pi a^2$,

$$\ln\left(\frac{\hbar^2}{2ma^2|E|}\right) \simeq \frac{2\hbar^2}{ma^2U_0},$$

$$E \simeq -\frac{\hbar^2}{2ma^2}\exp\left(-\frac{2\hbar^2}{ma^2U_0}\right).$$

Таким образом, в мелкой двумерной яме, как и в симметричной одномерной, всегда существует одно связанное состояние. Причем, как это видно из (2), глубина залегания соответствующего уровня энергии экспоненциально мала по сравнению с глубиной ямы. В трехмерной же яме связанное состояние есть не всегда (см. задачу 2.6.9).

17.2.10 Problems about motion in a magnetic field 1

(??? потом связи с кл мехом пропишу тоже в теории)
(!! очень скоро в 1 части добавлю формулы основные про это!!! почти готов, еще чуть прорешать задачи нужно)

Б-2.5.1 Частица в магнитном поле в декартовых координатах

Найти волновые функции и спектр энергии для заряженной частицы во внешнем однородном и постоянном магнитном поле, направленном по оси z. (Указание: использовать в качестве векторного потенциала A вектор с компонентами $\mathrm{A}_x = \mathrm{A}_z = 0$, $\mathrm{A}_y = \mathcal{H}x$.)

Определить число состояний, приходящихся на интервал $(p_z \div p_z + \Delta p_z)$ и один дискретный уровень, предполагая, что система заключена в ящик объема V (линейные размеры которого значительно больше ларморовского радиуса).

Solution.

Это известная задача про уровни Ландау, можно сразу написать ответ.

$$\hat{\mathrm{H}} = \frac{1}{2m}\left[\hat{\mathrm{p}}_x^2 + \left(\hat{\mathrm{p}}_y - \frac{e}{c}\mathcal{H}x\right)^2 + \hat{\mathrm{p}}_z^2\right]$$

$$\psi_{Ep_yp_z} = C\exp\left[\frac{i}{\hbar}(p_y y + p_z z)\right] f(x),$$

$$f(x): \qquad f''(x) + \frac{2m}{\hbar^2}\left[\left(E - \frac{p_z^2}{2m}\right) - \frac{m}{2}\omega_H^2(x - x_0)^2\right] f(x) = 0.$$

Здесь $\omega_H = \frac{e\mathcal{H}}{mc}(e > 0)$ и $x_0 = \frac{cp_y}{e\mathcal{H}}$. Решение уравнения (1) выражается через решение уравнения Шредингера для гармонического осциллятора с частотой ω_H (см. (II.18)). В итоге

$$\psi_{np_yp_z}(x, y, z) = C\exp\left[\frac{i}{\hbar}(p_y y + p_z z)\right] u_n^{\mathrm{osc}}\ (x - x_0),$$

$$E_{np_z} = \hbar\omega_H\left(n + \frac{1}{2}\right) + \frac{p_z^2}{2m}, \quad n = 0, 1, ...$$

Первое слагаемое в (2) описывает энергетические уровни поперечного движения (уровни Ландау). Они являются дискретными и нумеруются квантовым числом n. Движение вдоль поля не квантуется, квантовое число p_z может принимать значения $-\infty < p_z < \infty$. Уровни энергии (2) вырождены, ибо они не зависят от квантового числа p_y, которое также может изменяться от $-\infty$ до ∞.

Если ограничить область движения частицы ящиком в виде куба с ребром L, то p_z и p_y становятся дискретными:

$$p_i = \frac{2\pi\hbar}{L}n_i, \quad n_i = 0, \pm 1, ...$$

потому что предполагается граничное условие $\psi(x_i + L) = \psi(x_i)$. Исходя из того, что в классическом пределе на одно квантовое состояние (в одном измерении) приходится фазовый объем $2\pi\hbar$ (см. задачу 2.2.1) получим, что число квантовых состояний в объеме V в расчете на интервал Δp_z и на один дискретный уровень равно

$$\Delta N = \left(\frac{L}{2\pi\hbar}\right)^2 \Delta p_y \Delta p_z.$$

Из условия $0 < x_0 < L$ (центр классической орбиты внутри объема V, и радиус орбиты пренебрежимо мал по сравнению с L) имеем $\Delta p_y = e\mathcal{H}L/c$. Поэтому окончательно

$$\Delta N = \frac{e\mathcal{H}}{c}\frac{V}{(2\pi\hbar)^2}\Delta p_z$$

Б-2.5.2 Частица в магнитном поле в цилиндрических координатах

Найти уровни энергии и волновые функции заряженной бесспиновой частицы в однородном магнитном поле, направленном вдоль оси z, используя цилиндрическую систему координат.

Solution.

Это известная задача теории из книги Ландау, так можно обойти спецфункции, можно сразу написать ответ.

$$\mathbf{A} = \frac{1}{2}[\mathcal{H} \times \mathbf{r}].$$

$z \| \mathcal{H}$

$$\mathrm{A}_z = 0, \quad \mathrm{A}_\rho = 0, \quad \mathrm{A}_\varphi = \frac{1}{2}\mathcal{H}\rho.$$

Гамильтониан частицы массы M с зарядом $e (e > 0)$ имеет вид

$$\hat{\mathrm{H}} = \frac{1}{2M}\left(\hat{\mathcal{P}} - \frac{e}{c}\mathbf{A}\right)^2 = \frac{1}{2M}\hat{\mathcal{P}}^2 - \frac{e\hbar\mathcal{H}}{2Mc}\hat{I}_z + \frac{e^2\mathcal{H}^2}{8Mc^2}\rho^2.$$

$$\omega_H := e\mathcal{H}/(Mc) \qquad \hat{I}_z = -i\partial/\partial\varphi,$$

$$\hat{\mathrm{H}} = -\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial z^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right) + \frac{i}{2}\hbar\omega_H\frac{\partial}{\partial\varphi} + \frac{1}{8}M\omega_H^2\rho^2.$$

Гамильтониан (1)-(2) коммутирует с операторами $\hat{l}_z$ и $\hat{\mathrm{p}}_z$, поэтому решение стационарного уравнения Шредингера в цилиндрических координатах

$$\hat{\mathrm{H}}\psi(z,\rho,\varphi) = E\psi(z,\rho,\varphi)$$

следует искать в виде общей собственной функции трех операторов: $\hat{\mathrm{H}}$, $\hat{I}_z$ и $\hat{\mathrm{p}}_z$, т. е.

$$\psi(z,\rho,\varphi) = \psi_z(z)\Phi(\varphi)R(\rho),$$

$$\psi_z(z) \equiv \psi_{p_z}(z) = \frac{1}{\sqrt{2\pi h}}e^{\frac{i}{\hbar}p_z z}, \quad \Phi(\varphi) \equiv \Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}}e^{im\varphi}.$$

$$\psi(z,\rho,\varphi) = \frac{e^{im\varphi}}{\sqrt{2\pi}}\frac{e^{\frac{i}{\hbar}p_x z}}{\sqrt{2\pi\hbar}}R(\rho).$$

Для радиальной функции $R(\rho)$ получаем обыкновенное дифференциальное уравнение

$$-\frac{\hbar^2}{2M}\left(\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{dR}{d\rho} - \frac{m^2}{\rho^2}R\right) - \frac{1}{2}\hbar\omega_H mR + \frac{1}{8}M\omega_H^2\rho^2 R = E_H R.$$

(Мы представили полную энергию в виде суммы $E = E_z + E_H$, где $E_z = p_z^2/(2M)$ - энергия продольного движения частицы.) Потенциальная энергия в (4) зависит квадратично от переменной ρ, как и для гармонического осциллятора, поэтому ее удобно измерять в осцилляторных
единицах: $E_H = \hbar\omega_H\varepsilon$. Поделим уравнение (4) на $\hbar\omega_H$ и введем безразмерную переменную

$$\xi = \frac{\sqrt{2}\rho}{\rho_H} = \sqrt{\frac{2M\omega_H}{\hbar}}\rho,$$

где $\rho_H = \sqrt{\hbar/(M\omega_H)}$ - осцилляторная единица длины (II.16). В безразмерных переменных уравнение принимает вид

$$R'' + \frac{1}{\xi}R' + \left(\varepsilon - \frac{m^2}{\xi^2} + \frac{m}{2} - \frac{\xi^2}{16}\right)R = 0.$$

Выделим его асимптотики. При $\xi \to 0$ имеем

$$R_0'' + \frac{1}{\xi}R_0' - \frac{m^2}{\xi^2}R_0 = 0.$$

Ищем решение, как обычно, в виде степенной функкци $R_0 \sim \xi^s$ и получаем для s уравнение и его решение в виде

$$s(s-1) + s - m^2 = 0, \quad \to \quad s = \pm m.$$

Таким образом, асимптотика радиальной функции при $\xi \to 0$ есть

$$R|_{\xi\to 0} \sim \xi^{|m|}.$$

Для определения асимптотического решения при $\xi \to \infty$ на основании (5) получаем уравнение

$$R_\infty'' - \frac{1}{16}\xi^2 R_\infty = 0.$$

$$R_\infty \sim \mathrm{e}^{-\alpha\xi^2} \qquad \Rightarrow \qquad \alpha = 1/8,$$

$$R|_{\xi\to\infty} \sim e^{-\xi^2/8}.$$

Таким образом, полную радиальную функцию можно представить в виде

$$R(\xi) = e^{-\xi^2/8}\xi^{|m|}w(\xi),$$

учитывающем особенности поведения в нуле и на бесконечности. Подставляя функцию $R(\xi)$ в виде (6) в радиальное уравнение (5) и вводя новую переменную z согласно $z = \xi^2/4$, получим уравнение для функции $w(z)$:

$$z\frac{d^2w}{dz^2} + (|m| + 1 - z)\frac{dw}{dz} + \left[\varepsilon - \frac{|m| - m + 1}{2}\right]w = 0,$$

причем функцию $w(z)$ мы будем далее искать в виде суммы степенного ряда (вообще говоря, бесконечного)

$$\omega(z) = \sum_{k=0}^{\infty} a_k z^k.$$

Подставляя в (7) решение в виде суммы (8) и производя преобразование индекса суммирования таким образом, чтобы сгруппировать члены с одинаковыми степенями z, находим

$$\sum_{k=0}^{\infty} z^k \left[(k+1)(k+1+|m|)a_{k+1} + \left(\varepsilon - k - \frac{|m| - m + 1}{2}\right)a_k\right] = 0.$$

Для того, чтобы левая часть данного уравнения обратилась в ноль, необходимо и достаточно потребовать, чтобы коэффициенты при всех степенях z были бы равны нулю. На основании этого получаем рекуррентные соотношения для коэффициентов a_k:

$$a_{k+1} = a_k \frac{2k + |m| - m + 1 - 2\varepsilon}{2(k+1)(k+1+|m|)}.$$

Заметим, что в ряде (8) отношение двух последующих коэффициентов согласно (9) при $k \gg 1$ стремится к пределу

$$\left.\frac{a_{k+1}}{a_k}\right|_{k\gg 1} \to \frac{1}{k}$$

и будет таким же, как и у функции e^z, разложенной в ряд

$$e^z = \sum_{k=0}^{\infty} \frac{z^k}{k!}.$$

Поэтому при $z \to \infty$ мы получим $w(z) \sim e^z$ или $w(\xi) \sim e^{\xi^2/4}$, т. е. радиальная функция (6) при $\xi \to \infty$ будет экспоненциально расти: $R(\xi)|_{\xi\to\infty} \sim e^{\xi^2/8}$. Единственная возможность избежать данного неограниченного роста "оборвать" ряд (8) при некотором $k = n_\rho$ и превратить его в полином. При этом должно выполняться условие

$$\varepsilon_{n_\rho} = n_\rho + \frac{|m| - m + 1}{2}, \quad n_\rho = 0, 1, 2, ...$$

Число n_ρ, как и обычно, называется радиальным квантовым числом и определяет количество нулей многочлена $w_{n_\rho}(z)$.

Окончательно получаем энергетический спектр заряженной частицы в однородном магнитном поле:

$$E_{np_z} = \hbar\omega_H \left(n + \frac{1}{2}\right) + \frac{p_2^2}{2M}, \quad n = n_\rho + \frac{|m| - m}{2} = 0, 1, 2, ...$$

где мы ввели главное квантовое число n. Данный результат находится в полном согласии с формулой (2) решения задачи 2.5.1.

Уровни энергии (11) вырождены по значению проекции момента на направление магнитного поля: каждому фиксированному значению числа n отвечают состояния с

$$m = -n, -n + 1, ..., 0, 1, ...\infty.$$

(??? бесконечная кратность вырождения, можно что-то сказать про это????)

Для функции $w(z)$ мы получаем ряд (8), определяемый рекуррентными соотношениями (9) и сводящийся к вырожденной гипергеометрической функции $F(-n_\rho, |m| + 1, z)$, которая является регулярным при $z \to 0$ решением уравнения (7). При условии (10) гипергеометрическая функция превращается в присоединенный полнном Лагерра (см. (Д.24)), Т. е.

$$w_{n_\rho m}(z) = a_0 \left[1 - \frac{n_\rho}{(|m| + 1)}\frac{z}{1} + \frac{n_\rho (n_p - 1)}{(|m| + 1)(|m| + 2)}\frac{z^2}{2} + ...\right] =$$
$$= a_0 F(-n_\rho, |m| + 1, z) = \frac{a_0 |m|!}{(|m| + n_\rho)!} L_{n_\rho}^{|m|}(z).$$

Восстанавливая исходные обозначения, запишем общий вид радиальной функции $R(\rho)$, нормированной условием $\int\limits_0^\infty |R(\rho)|^2 \rho d\rho = 1$:

$$R_{n_\rho m}(\rho) = \frac{1}{\rho_H \sqrt{n_\rho! \, (|m| + n_\rho)!}} \exp\left(-\frac{\rho^2}{4\rho_H^2}\right) \left(\frac{\rho}{\sqrt{2}\rho_H}\right)^{|m|} L_{n_\rho}^{|m|}\left(\frac{\rho^2}{2\rho_H^2}\right)$$

Б-2.5.3 Факторизация волновой функции в магнитном поле

Показать, что в однородном магнитном поле, переменном во времени, волновая функция частицы со спином распадается на произведение координатной и спиновой функций.

Solution.

Утверждается, что координатные и спиновые переменные в уравнении Паули разделяются только в случае наличия однородного магнитного поля, возможно, зависящего от времени. Предполагая возможность такого разделения, ищем решение уравнения Паули

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}, t) = \left(\hat{\mathrm{H}}^\Psi - \mu_0(\sigma\mathcal{H})\right)\Psi(\mathbf{r}, t),$$

где

$$\hat{\mathrm{H}}^\Psi = \frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}\right)^2 + \hat{\mathrm{U}}(\mathbf{r}), \qquad \mu_0 = \frac{e\hbar}{2mc}, \quad e > 0,$$

в следующем виде:

$$\Psi(\mathbf{r}, t) = f(\mathbf{r}, t)\chi(t).$$

Здесь $\chi(t)$ - спиновая функция, зависящая только от времени. Подставим (2) в (1) и потребуем, чтобы функция $f(\mathbf{r}, t)$ подчинялась уравнению Шредингера для бесспиновой частицы

$$i\hbar\frac{\partial}{\partial t}f(\mathbf{r}, t) = \hat{\mathrm{H}}^\Psi f(\mathbf{r}, t).$$

Тогда для спиновой функции мы получим

$$i\hbar\frac{\partial}{\partial t}\chi(t) = -\mu_0(\hat{\sigma}\mathcal{H})\chi(t).$$

Уравнения (3) и (4) будут независимыми, если магнитное поле $\mathcal{H}$ - однородное, т. е. не зависит от координат.

Б-2.5.4

Найти зависимость от времени спиновой функции покоящегося мюона, если в начальный момент

$$\chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

и включается магнитное поле $\mathcal{H}$, направленное вдоль оси x. Найти $\langle\hat{\sigma}_x\rangle, \langle\hat{\sigma}_y\rangle, \langle\hat{\sigma}_z\rangle$ и убедиться, что магнитный момент мюона совершает прецессию вокруг магнитного поля. Получить вид спиновых операторов в представлении Гейзенберга.

Solution.

Суть решения в том, что 2.5.4. По условию задачи магнитное поле постоянное и однородное, поэтому переменные в уравнении Паули разделяются, и уравнение (4) задачи 2.5.3 принимает вид

$$i\hbar\frac{\partial}{\partial t}\chi(t) = -\hbar\Omega\hat{\sigma}_x\chi(t), \quad \Omega = \frac{e\mathcal{H}}{2mc}.$$

С учетом явного вида матрицы $\hat{\sigma}_x$ уравнение (1) переходит в

$$\frac{\partial}{\partial t}\begin{pmatrix} s_1(t) \\ s_2(t) \end{pmatrix} = i\Omega\begin{pmatrix} s_2(t) \\ s_1(t) \end{pmatrix}; \quad \chi(0) = \begin{pmatrix} s_1(0) \\ s_2(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

- начальное условие. Решаем далее систему дифференциальных уравнений для s_1 и s_2 и получаем

$$\chi(t) = \begin{pmatrix} \cos\Omega t \\ i\sin\Omega t \end{pmatrix}.$$

Используя (2), находим средние значения

$$\langle\hat{\sigma}_x\rangle = \chi^+\hat{\sigma}_x\chi = 0, \quad \langle\hat{\sigma}_y\rangle = \sin 2\Omega t, \quad \langle\hat{\sigma}_z\rangle = \cos 2\Omega t.$$

Поскольку $\langle\hat{\mu}\rangle_\chi = \mu_0\langle\hat{\boldsymbol{\sigma}}\rangle_\chi$, то ясно, что в плоскости yOz, перпендикулярной к направлению магнитного поля, происходят периодические во времени изменения средних значений магнитного момента мюона. Это интерпретируется, как прецессия магнитного момента вокруг направления магнитного поля.

Перейдем к представлению Гейзенберга. Из формулы (1) следует, что гамильтониан $\hat{\mathrm{H}} = -\hbar\Omega\hat{\sigma}_x$ н поэтому

$$\begin{aligned}
(\hat{\sigma}_x)_H &= e^{-i\Omega t\hat{\sigma}_x}\hat{\sigma}_x e^{i\Omega t\hat{\sigma}_x} = \hat{\sigma}_x, \\
(\hat{\sigma}_y)_H &= e^{-i\Omega t\hat{\sigma}_x}\hat{\sigma}_y e^{i\Omega t\hat{\sigma}_x} = \hat{\sigma}_y\cos 2\Omega t + \hat{\sigma}_z\sin 2\Omega t, \\
(\hat{\sigma}_z)_H &= e^{-i\Omega t\hat{\sigma}_x}\hat{\sigma}_z e^{i\Omega t\hat{\sigma}_x} = \hat{\sigma}_z\cos 2\Omega t - \hat{\sigma}_y\sin 2\Omega t.
\end{aligned}$$

При вычислении необходимо использовать соотношение $e^{i\Omega t\hat{\sigma}_x} = \cos\Omega t + i\hat{\sigma}_x\sin\Omega t$, а также свойства матриц Паули. Таким образом, в представлении Гейзенберга матрицы Паули (и спиновые операторы $\hat{\mathrm{s}}_i = \frac{1}{2}\hat{\sigma}_i$) изменяются во времени, как компоненты трехмерного вектора.

Б-2.5.5 Спин электрона в магнитном поле $\mathcal{H}$ в представлении Гейзенберга

Найти оператор спина электрона в однородном магнитном поле $\mathcal{H}$ в представлении Гейзенберга. Считать, что других взаимодействий, изменяющих спиновое состояние электрона, нет.

Solution.

Суть решения в том, что 2.5.5. Данную задачу можно решить двумя способами: 1) используя унитарное преобразование, связывающее представления Шредингера и Гейзенберга (II.11) и 2) непосредственно решая уравнения Гейзенберга (II.10). Первый способ был применен при решении задачи 2.5.4, здесь мы воспользуемся вторым способом.

Направим магнитное поле по оси z, тогда спиновый гамильтониан электрона в однородном магнитном поле примет вид

$$\hat{\mathrm{H}} = 2\mu_0\mathcal{H}\hat{\mathrm{s}}_2.$$

Здесь $\mu_0 = e\hbar/(2mc)$ - магнетон Бора, $-e < 0$ - заряд электрона. Для решения задачи воспользуемся уравнением Гейзенберга (1I.10). Получаем (с учетом $[\hat{\mathrm{s}}_2, \hat{\mathrm{s}}_\pm] = \pm\hat{\mathrm{s}}_\pm$)

$$\frac{d\hat{\mathrm{s}}_z}{dt} = 0, \quad \frac{d\hat{\mathrm{s}}_\pm}{dt} = \pm\frac{i}{h}2\mu_0\mathcal{H}\hat{\mathrm{s}}_\pm.$$

Полученные уравнения легко решаются:

$$\hat{\mathrm{s}}_z(t) = \hat{\mathrm{s}}_z, \quad \hat{\mathrm{s}}_\pm(t) = e^{\pm i\omega t}\hat{\mathrm{s}}_\pm,$$

где $\omega = 2\mu_0\mathcal{H}/\hbar$. Окончательно будем иметь (ср. с задачей 2.5.4)

$$\hat{\mathrm{s}}_x(t) = \hat{\mathrm{s}}_x\cos\omega t - \hat{\mathrm{s}}_y\sin\omega t,$$
$$\hat{\mathrm{s}}_y(t) = \hat{\mathrm{s}}_y\cos\omega t + \hat{\mathrm{s}}_x\sin\omega t.$$

Б-2.5.6, ЛШ-5 Спин во вращающемся поле

Частица со спином $s = 1/2$ и магнитным моментом μ находится в постоянном вертикальном и вращающемся горизонтальном магнитном полях

$$B = (B_1\cos\omega t, B_1\sin\omega t, B_0)$$

1) Запишите уравнение Шредингера в представлении взаимодействия, считая переменную часть поля «возмущением».
2) Решите уравнение и найдите S -матрицу.
3) Пусть при $t = 0$ частица находится в состоянии «спин вверх». Какова вероятность найти ее в состоянии «спин вниз» в момент $t > 0$?
4) Рассмотрите отдельно случай резонанса $\omega = 2\mu B_0$.

Обзор решения

Используем определение представления взаимодействия, а также матричный вид экспоненты от сигма-матриц. Для полученной системы вводим “вращающиеся” переменные, получаем общее решение. S-матрицу находим из определения, зная общее решение.

Уравнение Шредингера и S матрица

$\hat{\mathcal{H}} \equiv \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}}$,

$$\hat{\mathcal{H}}_0 = \mu B_0\sigma_z = \begin{pmatrix} \mu B_0 & 0 \\ 0 & -\mu B_0 \end{pmatrix},$$
$$\hat{\mathcal{H}}_{\text{int}} = \mu B_1\left(\sigma_x\cos\omega t + \sigma_y\sin\omega t\right) = \begin{pmatrix} 0 & \mu B_1 e^{-i\omega t} \\ \mu B_1 e^{i\omega t} & 0 \end{pmatrix}$$

$$\hat{\mathcal{H}}_{\text{int}}(t) = e^{i\hat{\mathcal{H}}_0 t}\hat{\mathcal{H}}_{\text{int}}\, e^{-i\hat{\mathcal{H}}_0 t} = \begin{pmatrix} e^{i\mu B_0 t} & 0 \\ 0 & e^{-i\mu B_0 t} \end{pmatrix}\hat{\mathcal{H}}_{\text{int}}\begin{pmatrix} e^{-i\mu B_0 t} & 0 \\ 0 & e^{i\mu B_0 t} \end{pmatrix} = \mu B_1\begin{pmatrix} 0 & e^{-2i\Omega t} \\ e^{2i\Omega t} & 0 \end{pmatrix},$$

$\Omega := \omega/2 - \mu B_0$.
$i\dot{\psi} = \hat{\mathcal{H}}_{\text{int}}(t)\psi$,

$$i\dot{\psi}_\uparrow = \mu B_1 e^{-2i\Omega t}\psi_\downarrow,$$
$$i\dot{\psi}_\downarrow = \mu B_1 e^{2i\Omega t}\psi_\uparrow$$

$$\varphi_\uparrow := e^{i\Omega t}\psi_\uparrow,$$
$$\varphi_\downarrow := e^{-i\Omega t}\psi_\downarrow.$$

Уравнения для $\varphi_\alpha(t)$ не содержат явной зависимости от времени:

$$i\dot{\varphi}_\uparrow + \Omega\varphi_\downarrow = \mu B_1\varphi_\uparrow,$$
$$i\dot{\varphi}_\downarrow - \Omega\varphi_\uparrow = \mu B_1\varphi_\downarrow,$$

или

$$i\dot{\varphi} = \begin{pmatrix} -\Omega & \mu B_1 \\ \mu B_1 & \Omega \end{pmatrix}\varphi.$$

Общее решение этих уравнений имеет вид (????)

$$\varphi(t) = c_+\begin{pmatrix} (1+\lambda)^{1/2} \\ -(1-\lambda)^{1/2} \end{pmatrix}e^{i\bar{\omega}t} + c_-\begin{pmatrix} (1-\lambda)^{1/2} \\ (1+\lambda)^{1/2} \end{pmatrix}e^{-i\bar{\omega}t},$$

где $\tilde{\omega} = \sqrt{\Omega^2 + (\mu B_1)^2}, \lambda = \Omega/\tilde{\omega}$, а коэффициенты $c_\pm$ определяются начальными условиями.

$\hat{S}(t):\quad \psi_i(t) \equiv \hat{S}(t)\psi_i(0)$, (???????)

$$\hat{S}(t) = \begin{pmatrix} e^{-i\Omega t} & 0 \\ 0 & e^{i\Omega t} \end{pmatrix} \begin{pmatrix} (1+\lambda)^{1/2} e^{i\tilde{\omega}t} & (1-\lambda)^{1/2} e^{-i\tilde{\omega}t} \\ -(1-\lambda)^{1/2} e^{i\omega\omega t} & (1+\lambda)^{1/2} e^{-i\tilde{\omega}t} \end{pmatrix} \cdot \frac{1}{2} \begin{pmatrix} (1+\lambda)^{1/2} & -(1-\lambda)^{1/2} \\ (1-\lambda)^{1/2} & (1+\lambda)^{1/2} \end{pmatrix} =$$
$$= \begin{pmatrix} W(t)e^{-i\Omega t} & -i\left(1-\lambda^2\right)^{1/2} e^{-i\Omega t} \sin\tilde{\omega}t \\ -i\left(1-\lambda^2\right)^{1/2} e^{i\Omega t} \sin\tilde{\omega}t & W^*(t)e^{i\Omega t} \end{pmatrix},$$

$W(t) := \cos\tilde{\omega}t + i\lambda \sin\tilde{\omega}t$.

(??? по идее тут возня будет с обращением матрицы. ну и по идее подставить просто в эту формулу и нужно, где первый член просто уже найден выше.)

Вероятность поворота спина

Рассмотрим теперь вероятность переворота спина. Ее можно найти с помощью S-матрицы, а можно и прямо из (2.26). Воспользуемся вторым способом. Поскольку при $t = 0$ имеем $\varphi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, то коэффициенты $c_\pm$в выражении (2.26) есть $c_+ = (1+\lambda)^{1/2}/2$, $c_- = (1-\lambda)^{1/2}/2$. То есть

$$\varphi_l(t) = \frac{1}{2}\sqrt{1-\lambda^2}\left(e^{-i\tilde{\omega}t} - e^{i\tilde{\omega}t}\right) = \frac{\mu B_1}{i\tilde{\omega}} \sin\tilde{\omega}t.$$

$$p_\downarrow(t) = |\varphi_\downarrow(t)|^2 = \frac{(\mu B_1)^2}{\Omega^2 + (\mu B_1)^2} \sin^2\tilde{\omega}t.$$

Случай резонанса

Если выполнено условие резонанса $\omega = 2\mu B_0$, то $\Omega = 0, \tilde{\omega} = \mu B_1$ и выражение для S-матрицы упрощается:

$$\hat{S}(t) = \begin{pmatrix} \cos\mu B_1 t & -i\sin\mu B_1 t \\ -i\sin\mu B_1 t & \cos\mu B_1 t \end{pmatrix}.$$

Соответственно, в этом случае вероятность переворота спина есть $p_\downarrow(t) = \sin^2\mu B_1 t$.

Solution. по Белоусову

Суть решения в том, что 2.5.6. Уравнение эволюции спина в лабораторной системе координат имеет вид (см. задачу 2.5.3)

$$i\hbar\frac{\partial}{\partial t}\chi(t) = \hat{\mathrm{H}}\chi(t) = -\mu_0(\hat{\sigma}\mathcal{H})\chi(t) = -\gamma(\hat{\mathbf{S}}\mathcal{H})\chi(t),$$

где $\gamma = e/(mc)$ - гиромагнитное отношение для спинового момента, $\hat{\mathbf{S}} = (\hbar/2)\hat{\sigma}$ - оператор спина. Здесь наряду с постоянным полем $\mathcal{H}_0$, направленным по оси z, имеется также поле $\mathcal{H}_1$, вращающееся в плоскости xOy с угловой скоростью $\omega = \omega\mathbf{k}$. Поэтому гамильтониан явно зависит от времени.

Перейдем в систему координат K', вращающуюся относительно лабораторной системы K с угловой скоростью $\boldsymbol{\omega}$. При этом спиновая функция подвергнется преобразованию, отвечающему повороту на угол ωt:

$$\chi' = e^{\frac{i}{2}(\boldsymbol{\omega}\hat{\sigma})t}\chi = e^{\frac{i}{\hbar}(\hat{\mathbf{S}}\boldsymbol{\omega})t}\chi.$$

Функция χ' будет удовлетворять преобразованному уравнению

$$i\hbar\frac{\partial}{\partial t}\chi'(t) = \hat{\mathrm{H}}'_{\mathrm{eli}}\chi'(t), \text{ где } \hat{\mathrm{H}}'_{\mathrm{efI}} = e^{\frac{i}{\hbar}(\hat{\mathbf{S}}\boldsymbol{\omega})t}\hat{\mathrm{H}}e^{-\frac{i}{\hbar}(\hat{\mathbf{S}}\boldsymbol{\omega})t} - (\hat{\mathbf{S}}\boldsymbol{\omega}).$$

С учетом явного вида гамильтониана

$$\hat{\mathrm{H}} = -\gamma\left[\mathcal{H}_1\left(\hat{\mathrm{S}}_x\cos\omega t + \hat{\mathrm{S}}_y\sin\omega t\right) + \mathcal{H}_0\hat{\mathrm{S}}_z\right]$$

$$\hat{\mathrm{H}}'_{\mathrm{eff}} = -\gamma\left(\hat{\mathbf{S}}\mathcal{H}'_{\mathrm{efi}}\right), \quad \mathcal{H}'_{\mathrm{eff}} = \left\{\mathcal{H}_1, 0, \mathcal{H}_0 + \frac{\omega}{\gamma}\right\}.$$

Таким образом, мы перешли к некоторому эффективному полю $\mathcal{H}'_{\text{eff},}$ но зато теперь наш гамильтониан $\hat{\text{H}}'_{\text{elf}}$ не зависит от времени.

В новой системе координат магнитное поле однородно и постоянно во времени. Магнитный момент частицы должен прецессировать вокруг направления магнитного поля (см. задачу 2.5.4). Перейдем теперь в представление Гейзенберга, учитывая, что $\partial\hat{\text{H}}'_{\text{eff}}/\partial t = 0$:

$$\chi_H = \chi'' = e^{\frac{i}{\hbar}\hat{H}'_{e\|'}\chi'} = e^{-\frac{i}{\hbar}\gamma\left(\hat{\mathbf{S}}\mathcal{K}'_{ef11}\right)t}\chi' = e^{\frac{i}{\hbar}(\hat{\mathbf{S}}\Omega)t}\chi'.$$

Как видно, переход к представлению Гейзенберга эквивалентен еще одному повороту - вокруг направления вектора $\Omega = -\gamma\mathcal{H}'_{\text{eff}}$ на угол Ωt. Спиновая функция χ'' не зависит от времени (как и должно быть), ибо новый вид уравнения эволюции:

$$i\hbar\frac{\partial}{\partial t}\chi''(t) = 0, \quad \text{потому что} \quad \hat{\text{H}}''_{\text{eff}} = 0.$$

В итоге решение исходного уравнения $\chi(t)$ записывается при помощи оператора эволюции, представляющего собой два последовательных поворота. Поскольку $\chi''(t) = \chi''(0) = \chi'(0) = \chi(0)$, решение принимает вид

$$\chi(t) = e^{-\frac{i}{\hbar}(\hat{\mathbf{S}}\boldsymbol{\omega})t}e^{-\frac{i}{\hbar}(\hat{\mathbf{S}}\Omega)t}\chi(0).$$

Введем обозначения

$$\begin{cases} \omega_0 = \gamma\mathcal{H}_0, \omega_1 = \gamma\mathcal{H}_1, \\ \Omega = \sqrt{(\omega+\omega_0)^2 + \omega_1^2}, \end{cases} \qquad \begin{cases} \sin\theta = \frac{\mathcal{H}_1}{\mathcal{K}'_{\text{eff}}} = \frac{\omega_1}{\Omega}, \\ \cos\theta = \frac{\mathcal{H}_0+\omega/\gamma}{\mathcal{H}'_{\text{eff}}} = \frac{\omega+\omega_0}{\Omega}, \end{cases}$$

где θ - угол между векторами $\mathcal{H}_0$ и $\mathcal{H}'_{\text{eff.}}$. Тогда

$$(\hat{\mathbf{S}}\omega) = \omega\hat{\text{S}}_z, \quad (\hat{\mathbf{S}}\Omega) = -\Omega\left(\hat{\text{S}}_x\sin\theta + \hat{\text{S}}_z\cos\theta\right).$$

Вероятность переворота спина к моменту t равна

$$W_\chi\left(s_z = -\frac{1}{2}\right) = |\chi^+_{-1/2}\chi(t)|^2 = \sin^2\theta\sin^2\left(\frac{\Omega t}{2}\right) = \frac{\omega_1^2}{(\omega+\omega_0)^2+\omega_1^2}\sin^2\left[\frac{1}{2}\sqrt{(\omega+\omega_0)^2+\omega_1^2}\,t\right].$$

Вероятность переворота спина имеет резонансный характер. При условии $\mathcal{H}_1 \ll \mathcal{H}_0\,(\omega_1 \ll \omega_0)$ она мала при всех значениях частоты ω кроме узкой области вблизи точки резонанса $\omega \to -\omega_0 = -2\mu_0\mathcal{H}_0/\hbar$. В резонансной области вероятность может быть близкой к единице в некоторые моменты времени t.

Б-2.5.7 Измерение магнитного момента по создаваемому им полем (!??!)

Можно ли определить магнитный момент μ свободного электрона на основании измерения напряженности создаваемого им поля? (Использовать соотношение неопределённостей).

Solution.

Суть решения в том, что

2.5.7. Магнитное поле движущегося электрона обусловлено как его собственным магнитным моментом, так и его движением. Поле спинового магнитного момента - поле магнитного диполя $\mathcal{H}_{\text{сп}} \sim \mu/r^3$. Магнитное поле движущегося заряда ($v \ll c$)

$$\mathcal{H}_{\text{оp 6}} \sim |\frac{1}{c}[\mathbf{v}\times\mathcal{E}]| \sim \frac{v}{c}\frac{e}{r^2} \sim \frac{p}{mc}\frac{e}{r^2}.$$

Для реализации эксперимента необходимо выполнение условия

$$\frac{\mathcal{H}_{\text{оp}}}{\mathcal{H}_{\text{сп}}} \ll 1, \quad \text{т. е.} \quad \frac{p}{mc}\frac{e}{\mu} \ll 1.$$

Но импульс движущегося электрона точно не известен. Если считать, что область локализации электрона $\sim \Delta r$, то в соответствии с соотношением неопределённостей $p_{\min} \gtrsim \hbar/\Delta r$, и тогда получим

$$\Delta r \gg \frac{e\hbar}{mc}\frac{r}{\mu}.$$

Если μ - спиновый магнитный момент свободного электрона, то $\mu = \mu_0 = e\hbar/(2mc)$, следовательно $\Delta r \gg r$, что противоречит разумной постановке опыта, ибо для проведения эксперимента требуется $\Delta r \ll r$ - локализация частицы.

Б-2.5.8 Квантование магнитного поля в сверхпроводнике

В сверхпроводнике проделано цилиндрическое отверстие, в котором существует магнитное поле, параллельное оси цилиндра. (В толщу сверхпроводника магнитное поле не проникает). Показать, что поток магнитного поля внутри отверстия должен принимать дискретные значения. Найти квант магнитного потока.

Solution.

Это известная задача сверхпроводимости, можно сразу записать ответ.

$$\psi \equiv \sqrt{n_s} e^{i\varphi},$$

где $n_s(\mathbf{r})$ - плотность сверхпроводящих электронов, $\varphi(\mathbf{r})$ - фаза, общая для всех частиц, находящихся в сверхпроводящем состоянии. Используем выражение для плотности тока вероятности при наличии магнитного поля $\mathcal{H} = \operatorname{rot} \mathbf{A}$:

$$\mathbf{j} = \frac{i\hbar}{2m}\left[(\nabla\psi^*)\,\psi - \psi^*(\nabla\psi)\right] - \frac{e\mathbf{A}}{mc}\psi^*\psi = \left[\frac{\hbar}{m}\nabla\varphi - \frac{e}{mc}\mathbf{A}\right] n_s,$$

где мы учли вид функции (1). Проинтегрируем (2) по замкнутому контуру l, проходящему глубоко внутри сверхпроводника, полагая, что плотность n_s постоянна на контуре интегрирования:

$$\frac{mc}{en_s}\oint_l (\mathbf{j}d\mathbf{l}) = \frac{\hbar c}{e}\oint_l (\nabla\varphi d\mathbf{l}) - \oint_l (\mathbf{A}d\mathbf{l}).$$

Левая часть (3) обращается в нуль, так как в толще сверхпроводника магнитного поля нет, т. е. $\mathcal{H} = 0$, следовательно $\operatorname{rot} \mathcal{H} = \frac{4\pi}{c} j = 0$, поэтому и $\mathbf{j} = 0$. Далее

$$\oint_l (\mathbf{A}d\boldsymbol{l}) = \iint \operatorname{rot} \mathbf{A} d\mathbf{S} = \iint \mathcal{H} d\mathbf{S} = \Phi,$$

где Ф - поток вектора магнитного поля сквозь площадь, окруженную контуром. Н наконец

$$\oint_l (\nabla\varphi dl) = \oint \frac{d\varphi}{dl} dl = \oint d\varphi = 2\pi n, \quad n = 0, \pm 1, ...$$

где использовано условие однозначности волновой функции, вследствие чего изменение фазы должно быть равно $2\pi n$. Окончательно получаем, что

$$\Phi = n\Phi_0, \quad \Phi_0 = \frac{2\pi hc}{e},$$

где Φ_0 - квант магнитного потока.

ГК-4.1.

В однородном магнитном поле электрон, рассматриваемый согласно классической механике, движется по винтовой линии, ось которой направлена вдоль магнитного поля. Движение в плоскости, перпендикулярной магнитному полю, происходит с частотой, равной удвоенной частоте Лармора $\left(\omega = \frac{e\mathscr{E}}{2\mu c}\right)$. Рассмотрим движение волнового пакета на основании квантовой механики. Уравнение Шредингера для частицы в магнитном поле можно записать в сле,іующем виде:

$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2i}\Delta\Psi^* + \frac{\hbar}{i}\omega\left(x\frac{\partial\Psi}{\partial y} - y\frac{\partial\Psi}{\partial x}\right) + \frac{1}{2}u\left(\omega^2\left(x^2+y^2\right)\Psi^*\right.$

Чтобы найти решение задачи, удобно перейти к врашающейся системе координат

$$\left.\begin{array}{rl} x & = x'\cos\omega t' - y'\sin\omega t', \\ y & = x'\sin\omega t' + y'\cos\omega t', \\ z & = z', \\ t & = t', \\ \Psi(x,y,z,t) = & = \Psi'\left(x', y', z', t'\right) \end{array}\right\}$$

Тогда

$$\frac{\partial}{\partial t'} = \frac{\partial}{\partial t} + \omega\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right), \quad \Delta' = \Delta$$

Уравнение Шредингера в новых переменных принимает след ую у ylo форМу:

$$i\hbar\frac{\partial\Psi'}{\partial t'} = -\frac{h^2}{2u'}\Delta'\Psi' + \frac{\mu\omega^2}{2}\left(x'^2 + y'^2\right)\Psi'$$

Решение этого уравнения может быты получено разделением переменных x', y', z'. Уравнение для функции о z') описывает свободное движение вдоль оси z. Решение уравнения, определяющее функцию $\psi(x, y, t)$, имеет вид

$$\psi(x, y, t) = \sum_{nm} A_n \left(x'\sqrt{\frac{\mu\omega\omega}{h}}\right)\gamma m\left(y'\sqrt{\frac{\mu\omega}{\hbar}}\right)e^{-i\omega t(n\div m-1)}$$

Здесь x' и y' функции координат x, y и временн, определяемые из (1), χ_n - собственные функции гармонического осцнліятора, A_{mm} - коэффициенты, подобранные так, чтобы выполнялось начальное условие. Это выражение пля $\psi(x, y, t)$ меняет лишь знак, если t возрастает на период классического движения $T = \frac{\pi}{\omega}$. Действительно, x' и y' при этом меняет знак и, учитывая свойство собственной функции осциллятора

$$\chi_n(-\xi) = (-1)^n\chi_n(\xi),$$

Получим:

$$\psi\left(x, y, t + \frac{\pi}{\omega}\right) = \sum A_{nm}(-1)^n\chi_n\left(x'\sqrt{\frac{\mu\omega}{\hbar}}\right)(-1)^m\chi_m\left(y'\sqrt{\frac{\mu\omega}{\hbar}}\right)e^{-i\omega t(n+m+1)}e^{-i\pi(n+m+1)} = -\psi(x, y, t).$$

Таким образом, в плоскости, перпендикулярной магнитному полю, волновой пакет будет периодически изменять свою форму с периодом, равным периоду классического движения частицы в магнитном поле. В направлении магнитного поля пакет расплывается точно так же, как и для свободного движения. Волновая функция $\psi(x, y, t)$ может быть иайдена в явном виде, если начальная функция задана в форме

$$\psi(x, y, 0) = e^{-\frac{\alpha^2}{2}\left[(x-x_0)^2+(y-y)^2\right]+\frac{ip_{0x}}{\hbar}x+\frac{ip_{0y}}{\hbar}}.$$

Полагая все $A_{nm} = 0$, за исключением $A_{00} = 1$, находим, что такой волновой пакет не расплывается в плоскости xy, а его центр тяжести описывает классическую траекторию.

ГК-4.2

2. Показать, что в случае наличия магнитного поля для операторов компонент скорости имеют место следующие правила коммутации:

$$\hat{v}_x\hat{v}_y - \hat{v}_y\hat{v}_x = \frac{ie\hbar}{\mu^2 c}\mathscr{H}_z;$$
$$\hat{v}_y\hat{v}_z - \hat{v}_z\hat{v}_y = \frac{ie\hbar}{\mu^2 C}\mathscr{H}_x;$$
$$\hat{v}_z\hat{v}_x - \hat{v}_x\hat{v}_z = \frac{\mathrm{ieh}}{\mu^2 c}\mathscr{H}_y.$$

Solution.

Для нахождения оператора $\hat{j}$ надо прокоммутировать вектор $\boldsymbol{r}$ с гамильтонианом

$$\hat{\boldsymbol{v}} = \frac{l}{\hbar}(\hat{H}r - r\hat{H})$$

так как

$$\hat{H} = \frac{1}{2\mu}\left(\hat{p} - \frac{e}{c}A\right)^2 + U(r),$$

то находим:

$$\mu\hat{\mathfrak{v}} = \left(\hat{p} - \frac{e}{c}A\right)$$

Теперь найдем правила коммутации этих операторов

$$\hat{v}_x\hat{v}_y - \hat{v}_y\hat{v}_x = \frac{e}{\mu^2 c}\left[-\left(\hat{p}_x A_y - A_y\hat{p}_x\right) + \left(\hat{p}_y A_x - A_x\hat{p}_y\right)\right] = \frac{ie\hbar}{\mu^2 c}\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) = \frac{ie\hbar}{\mu^2 c}\mathscr{H}_z.$$

Путем циклической перестановки получаем остальные два соотношения.

ГК-4.3

3. Основываясь на результатах задач 2 § 6 и 5§1, определить энергию заряженной частицы, движущейся в постоянном магнитном поле.

Solution.

Направим ось z по направлению магнитного поля, напряженность которого обозначим через $\mathscr{H}$. Компоненты скорости частицы удовлетворяют следующим правилам коммутации (см. задачу 2$6):

$$\hat{v}_x\hat{v}_y - \hat{v}_y\hat{v}_x = \frac{ie\hbar}{\mu^2 c}\mathscr{H}, \quad \hat{v}_y\hat{v}_z - \hat{v}_z\hat{v}_y = 0, \quad \hat{v}_z\hat{v}_x - \hat{v}_x\hat{v}_z = 0$$

Оператор энергии равен

$$\hat{H} = \frac{\mu\hat{v}_{\boldsymbol{x}}^2}{2} + \frac{\mu\hat{v}_{\vartheta}^2}{2} + \frac{\mu\hat{v}_z^2}{2}.$$

Представим H в виде суммы двух коммутирующих операторов

$$\hat{H}_1 = \frac{\mu\hat{v}_{\boldsymbol{x}}^2}{2} + \frac{\mu\hat{v}_y^2}{2}, \quad \hat{H}_2 = \frac{\mu\hat{v}_z^2}{2}.$$

Собственные значения $\hat{H}$ равны сумме собственных значений $\hat{H}_1$ и $\hat{H}_2$. Найдем собственные значения $\hat{H}_1$. Для этого введем новые обозначения $\hat{v}_x = \alpha\hat{Q}, \quad \hat{v}_y = \alpha\hat{P}$, где $\alpha = \sqrt{\frac{el\sigma\mathscr{L}}{\mu^2 c}}\cdot B$ переменных $\hat{P}, \hat{Q}$ правило коммутации имеет вид $\hat{P}\hat{Q} - \hat{Q}\hat{P} = -i$, а оператор $\hat{H}_1 = \hbar\frac{e\mathscr{C}}{2\mu c}\times\ \chi\left(\hat{P}^2 + \hat{Q}^2\right)$. На основании задачи 5&1 собственные значения $\hat{H}_1$

$$E_{1n} = \hbar\frac{e\mathscr{O}\mathcal{H}}{\mu c}(n + 1/2) \quad (n = 0, 1, 2, ...).$$

Собственные значения $\hat{H}_2$ образуют непрерывный спектр. Итак, энергия движения в магнитном поле

$$E_{nv_z} = \hbar\frac{e\mathscr{H}}{\mu c}(n + 1/2) + \frac{\mu v_z^2}{2}.$$

ГК-4.4

4. Определить энергетический спектр заряженной частицы, движущейся в однородном электрическом и однородном магнитном полях, направления напряженностей которых взаимно перпендикулярны.

Solution.

Направим ось z по направлению магнитного поля, а ось x вдоль электрического поля. Векторный потенциал магнитного поля возьмем в виде $A_y =$ e $x, A_x = A_z = 0$. Оператор Гамильтона в этом случае запишется следующим образом:

$$\hat{H} = \frac{\hat{p}_x^2}{2\mu} + \frac{\left(\hat{p}_y - \frac{e}{c}\mathscr{H}x\right)^2}{2\mu} + \frac{\hat{p}_z^2}{2\mu} - e\mathscr{E}x.$$

Вводя обозначение

$$\frac{e\mathscr{A}}{c}x - \hat{p}_y - \frac{\mu\cdot\mathcal{E}}{\mathscr{E}} = \hat{\pi},$$

получим для $\hat{H}$ выражение

$$\hat{H} = \frac{\hat{p}_x^2}{2\mu} + \frac{\hat{\pi}^2}{2\mu} - \frac{\hat{p}_y c\mathscr{E}}{\mathscr{C}} - \frac{\mu c^2\mathscr{G}^2}{2\mathscr{E}\mathcal{C}^2} + \frac{\hat{p}_z^2}{2\mu}.$$

Соотношение коммутации между $\hat{p}_x$ и $\hat{\pi}$

$$\hat{p}_{x^\pi} - \hat{\pi}\hat{p}_x = -i\frac{\hbar e_{\mathscr{A}}}{c}.$$

Отсюда находим, чго собственные значения оператора $\hat{H}_1 = \frac{\hat{p}_:^2}{2\mu} + \frac{\hat{\pi}^2}{2\mu}$ совпадают с уровнями энергии осциллятора, колеблющегося с удвоенной частотой Лармора

$$E_{1n} = \hbar\frac{e\mathscr{E}}{\mu c}(n + 1/2).$$

Поскольку операторы $\hat{p}_y$ и $\hat{p}_z$, входящие в последние слагаемые оператора Гамильтона, коммугируют с $\hat{H}_1$, оператор $\hat{H}_2 = \frac{\hat{p}_z^2}{2\mu} - \frac{\hat{p}_y c\mathscr{G}}{\mathscr{E}} - \frac{\mu c^2\mathscr{E}^2}{2\mathscr{C}^2}$ может быть приведен одновременно с $\hat{H}_1$ к диаготальному виду.

Итак, энергетический спектр частицы

$$E_{np_yp_z} = \hbar\frac{e\mathscr{C}}{\mu c}(n + 1/2) + \frac{p_z^2}{2\mu} - \frac{p_y c\mathscr{E}}{\mathscr{E}} - \frac{\mu c^2\mathscr{G}^2}{2\mathscr{C}^2}.$$

Сравнение с результатом предыдущей задачи показывает, что электрическое поле снимает вырождение, которое имеет место в случае одного только магнитного поля: энергетические уровни при наличии электрического поля зависят от трех квантовых чисел.

ГК-4.5

5. Определить волновые функции заряженной частицы при движении во взаимно перпендикулярных однородных магнитном и электрическом полях.

Solution.

$$\psi_{np_yp_z}(x, y, z) = e^{\frac{i}{\hbar}(py^{y+p_z})}e^{-\frac{e\mathscr{H}}{2\hbar c}\left(x-\frac{cp_y}{e\mathscr{C}C}-\frac{\mu c^2\mathscr{E}}{e\mathscr{C}}\right)^2} H_n\left[\sqrt{\frac{egt}{ch}}\left(x - \frac{cp_y}{e^2t} - \frac{\mu c\mathscr{G}}{eg^2}\right)\right].$$

$$E_{nmk} = \hbar\sqrt{\omega^2 + \omega_0^2}(2n + |m| + 1) + \hbar\omega m + \hbar\omega_0(k + 1/2),$$

где

$$\omega = \frac{e\mathscr{C}}{2\mu c} \quad (n = 0, 1, 2, ..., m = 0, \pm1, \pm2, ...,$$
$$k = 0, 1, 2, ...).$$

17.2.11 Problems about motion in a magnetic field 2

ГК-4.7.

Определить зависящие от времени операторы координат $\hat{x}, \hat{y}$ заряженной частицы, движущейся в однородном магнитном поле (векторный потенциал $A_x = -\frac{\mathscr{H}}{2}y$, $A_y = \frac{\mathscr{H}}{2}x$, $A_z = 0$). Найти $\overline{(\hat{x} - \bar{\hat{x}})^2}$ и $\overline{(\hat{y} - \bar{\hat{y}})^2}$ как функции времени.

Solution.

$$\hat{x}(t) = \left(\frac{i\hbar}{\mu\omega}\frac{\partial}{\partial y} + \frac{x}{2}\right)\cos\omega t + \left(-\frac{i\hbar}{\mu\omega}\frac{\partial}{\partial x} + \frac{y}{2}\right)\sin\omega t + \left(-\frac{i\hbar}{\mu\omega}\frac{\partial}{\partial y} + \frac{x}{2}\right).$$

$$\hat{y}(t) = \left(-\frac{i\hbar}{\mu\omega}\frac{\partial}{\partial y} - \frac{x}{2}\right)\sin\omega t + \left(-\frac{i\hbar}{\mu\omega}\frac{\partial}{\partial x} + \frac{y}{2}\right)\cos\omega t + \left(-\frac{i\hbar}{\mu\omega}\frac{\partial}{\partial x} + \frac{y}{2}\right).$$

Здесь $\omega = \frac{eH}{\mu c}$ (удвоенная частота прецессии Лармора).

ГК-4.8

Определить уровни энергии и волновые функции заряженной частицы, движущейся в однородном магнитном поле. Воспользоваться цилиндрической системой координат. Векторный потенциал взять в форме $A_\varphi = \frac{\mathscr{H}}{2}\rho, A_\rho = A_z = 0$.

Solution.

Уравнение Шредингера в цилиндрических координатах ρ, φ, z имеет вид (??????)

$$-\frac{\hbar^2}{2\mu}\left\{\frac{\partial^2\psi}{\partial z^2}+\frac{\partial^2\psi}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial\cdot}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2\nu}{\partial\varphi^2}\right\}=\frac{ie\hbar}{2\mu c}e\theta\frac{\partial\psi}{\partial\varphi}+\frac{e^2g\ell^2}{8\mu c^2}\rho^2\Big]=E\psi.$$

Решение ищем в форме

$$\psi(\rho,\varphi,z)=\frac{1}{\sqrt{2\pi}}R(p)e^{ik_zz}e^{im\varphi}.$$

Обозначим через γ и β величины

$$\gamma=\frac{e\mathscr{H}}{2ch},\quad \beta=\frac{2\mu E}{\hbar^2}-k_z^2$$

В уравнение, определяющее радиальную функцию $R(p)$,

$$R''+\frac{1}{\rho}R'+\left(\beta--\gamma^2\rho^2-2\gamma m-\frac{m^2}{\rho^2}\right)R=0$$

введем новую независимую переменную $\xi=\gamma\rho^2$, тогда

$$\xi R''+R'+\left(-\frac{\xi}{4}+\lambda-\frac{m^2}{4\xi}\right)R=0,$$

где $\lambda=\frac{\beta}{4\gamma}-\frac{m}{2}$. Искомая функция при $\xi\to\infty$ ведет себя как $e^{-\xi/2}$, а при малых ξ пропорииональна $\xi^m|/2$. Решение дифференциального уравнения (1) ищем в виде

$$R=e^{-\xi/2\xi|m|/2}w(\xi).$$

Функция $w(\xi)$ находится из уравнения

$$\xi\omega''+(1+|m|-\xi)w'+\left(\lambda-\frac{|m|+1}{2}\right)w=0,$$

решение которого представляет вырожденную гипергеометрическую функцию:

$$w=F\left\{-\left(\lambda-\frac{|m|+1}{2}\right),|m|+1,\xi\right\}.$$

Для того чтобы волновая функция была конечна, величина $\lambda-\frac{|m|+1}{2}$ должна равняться целому неотрицательному числу n. Таким образом, уровни энергии определяются выражением

$$E=h\frac{e\mathscr{H}C}{\mu c}\left(n+\frac{|m|}{2}+\frac{m}{2}+\frac{1}{2}\right)+\frac{l_1^2k_z^2}{2\mu}$$

ГК-4.9

9. Найти компоненты плотности тока для заряженной частицы, движущейся в однородном магнитном поле для состояния, характеризуемого квантовыми числами n, m, k_z (см. предыдущую задачу).

Solution.

В цилиндрических координатах

$$\begin{aligned}J_{\mathrm{p}}&=0,\\ J_\varphi&=\left(\frac{e\hbar m}{\mu\rho}-\frac{e^2\mathscr{H}}{2\mu c}p\right)|\psi_{nmk_z}|^2,\\ J_z&=\frac{e\hbar\bar{k_z}}{\mu}|\psi_{nmk_z}|^2.\end{aligned}$$

ГК-10

10. Найти в квазиклассическом приближении уровни энергии заряженной частицы, находящейся в однородном магнитном поле (цилиндрические координаты).

Solution.

Уравнение для радиальной волновой функции R подстановкой $u = \sqrt{\rho}R$ приводится к виду

$$u'' + \left[\frac{2i}{h^2}E - k_z^2 - \frac{1}{p^2}\left(m + \frac{e\mathscr{H}C}{2\hbar c}p^2\right)^2\right]u = 0,$$

при этом $m^2 - \frac{1}{4}$ заменяется на m^2*. Эта замена аналогична замене $l(l+1) \to (l+1/2)^2$ и может быть обоснована способом, указанным при решении задачи 2$5. (??)

Выражение

$$U_{\text{eff}}(\rho) = \frac{\hbar^2}{2\mu p^2}\left(m + \frac{e\mathscr{H}}{2\hbar c}p^2\right)^2$$

можно рассматривать как эффективную потенциальную энергию при одномерном движении.

Из условия квантования (!!! укажу еще раз этот крутой метод в 1 части!!!!)

$$\int_{p_1}^{\rho_2}\sqrt{\frac{2p}{\hbar^2}E - k_z^2 - \frac{1}{p^2}\left(m + \frac{e^g\mathscr{G}}{2\hbar c}p^2\right)^2}\,dp = \pi(n+1/2)$$

получаем энергетический спектр:

$$E - \frac{\hbar^2 k_z^2}{2\mu} = \frac{e\hbar\mathscr{C}}{\mu c}\left(n + \frac{|m|}{2} + \frac{m}{2} + \frac{1}{2}\right).$$

Энергия, отсчитываемая от минимума $U_{\text{eff}}(p)$ равна

$$E' = \frac{eh\mathscr{H}}{\mu c}(n+1/2)$$

представляет собою энергию радиального движения, а энергия

$$E'' = \frac{e\hbar\mathscr{H}}{2\mu c}(m + |m|)$$

соответствует энергии вращательного движения. Переход к классическим круговым орбитам осуществляется при выполнении условия $E' \ll E''$ или $n \ll \frac{m+|m|}{2}$. Это условие, очевидно, выполняется лишь при положительных m и поэтому может быть записано в виде $n \ll m$.

ГК-4.11

11. Определить классически доступную область радиального движения частицы в магнитном поле (см. предыдущую задачу).

Solution.

Приравнивая нулю подкоренное выражение, получаем для $m > 0$

$$p_{1,2} = \sqrt{\frac{2\hbar c}{e_Q\mathscr{F}}}\left(\sqrt{n + m + \frac{1}{2}} \pm \sqrt{n + \frac{1}{2}}\right).$$

ГК-4.12 Размазанность орбиты (???)

Оценить минимальную «размазанность» орбиты в радиальном направлении для заряженной частицы в магнитном поле.

Solution.

(???)

$$\Delta p \sim \sqrt{\frac{\hbar c}{e\mathscr{H}}}.$$

ГК-4.13 (???)

Уравнение Паули имеет вид

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = \hat{H}_0\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} - \mu_0(\hat{\sigma}\,\mathcal{H})\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix},$$

где $\hat{H}_0 = \frac{1}{2\mu}\left(p - \frac{e}{c}A\right)^2 + eU,$ а μ_0 - магнитный момент частицы. Будем искать волновую функцию в виде

$$\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = \varphi(x,y,z,t)\begin{pmatrix}s_1(t)\\ s_2(t)\end{pmatrix}.$$

где функция φ является решением уравнения $i\hbar\frac{\partial\varphi}{\partial t} = \hat{H}_0\varphi$.

Тогда для спиновой функции $\begin{pmatrix}s_1\\ s_2\end{pmatrix}$ получаем уравнение

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}s_1\\ s_2\end{pmatrix} = -\mu_0(\hat{\boldsymbol{\sigma}}\boldsymbol{\mathcal{H}})\begin{pmatrix}s_1\\ s_2\end{pmatrix}.$$

ГК-4.15

Поскольку $\mathscr{H}_x = \mathscr{H}_y = 0$, $\mathscr{H}_z = \mathscr{H}C'(t)$, имеем:

$$i\hbar\frac{\partial s_1}{\partial t} = -\mu_0\mathscr{H}(t)s_1,$$
$$i\hbar\frac{\partial s_2}{\partial t} = \mu_0\mathscr{H}(t)s_2.$$

Решения этих уравнений имеют вид

$$s_2 = c_2 e^{-\frac{i_2,2}{\hbar}\int\limits_0^t \mathscr{H}(t)dt.}$$

Постоянные c_1 и c_2 находим из начальных условий: $c_1 = e^{-i\alpha}\cos\delta, c_2 = e^{i\alpha}\sin\delta$. Из вида функции s_1 и s_2 следует, что вероятность той или иной ориентации спина на ось z не меняется со временем. Среднее значение проекции спина на ось x определяется выражением

$$\bar{\hat{s}}_x = -\frac{\hbar}{2}\sin 2\hat{\delta}\cdot\cos\left\{\frac{2\mu_0}{\hbar}\int\limits_0^t \mathscr{H}(t)dt - 2\alpha\right\}$$

и аналогично

$$\overline{\hat{s}_y} = -\frac{\hbar}{2}\sin 2\hat{o}\cdot\sin\left\{\frac{2\mu_0}{\hbar}\int\limits_0^t \mathscr{H}(t)dt - 2x\right\}.$$

Направление, вдоль которого проекция спина имеет значение $+1/2$, характеризуется полярными координатами $\theta = 2\hat{,}\ \Phi = 2\left(\alpha - \frac{\mu_0}{\hbar}\int\limits_0^t \mathscr{H}(t)dt\right)$. Таким образом, это направление

$$s_1 = c_1 e^{\frac{iw_0}{\hbar}\int\limits_0^t \mathscr{H}(t)dt}$$

описывает с течением времени коническую поверхность. При постоянной напряженности поля прямая, «вдоль которой направлен спин», равномерно вращается вокруг направления магнитного поля частотой $\frac{2\mu_0\mathscr{H}}{h}$.

ГК-4.16

Состояние с произвольной поляризацией падающего пучка всегда может быть представлено как суперпозиция двух состояний, в одном из которых $\begin{pmatrix}1\\0\end{pmatrix}$ спин направлен вдоль оси z, а в другом $\begin{pmatrix}0\\1\end{pmatrix}$ в противоположном направлении. Рассмотрим сначала случай, когда спины нейтронов в падающем пучке направлены по оси z. Тогда падающая, отраженная и преломленная волны будут иметь вид

$$A\begin{pmatrix}1\\0\end{pmatrix}e^{ikr},\quad B\begin{pmatrix}1\\0\end{pmatrix}e^{ik_1r},\quad C\begin{pmatrix}0\\1\end{pmatrix}e^{ik_2r}.$$

Величины $\boldsymbol{k},\boldsymbol{k}_1,\boldsymbol{k}_2$ связаны с полной энергией E и магнитным моментом μ_0 нейтрона соотношениями:

$$\boldsymbol{k}=\frac{\boldsymbol{p}}{h},\quad \frac{\hbar^2k^2}{2\mu}=E,\quad \frac{\hbar^2k_1^2}{2\mu}=E,\quad \frac{\hbar^2k_2^2}{2\mu}=E+\mu_0\Theta^3.$$

Из условия непрерывности на плоскости раздела ($x=0$) вопновой функции и ее производной по x следует:

$$k_y=k_{1y}=k_{2y},\quad k_z=k_{1z}=k_{2z},$$
$$A+B=C,$$
$$k_xA+k_{1x}B=k_{2x}C.$$

Из этих соотношений вытекает, что $k_{1x}=-k_x$, т. е. угол падения ϕ равен углу отражения ϕ_1. Положим для простоты $k_y=0$. Решая уравнения, находим:

$$\left(\frac{B}{A}\right)=\frac{k_x-k_{2x}}{k_x+k_{2x}}\quad\left(\frac{C}{A}\right)=\frac{2k_x}{k_x+k_{2x}},$$
$$k_{2x}=k_x\sqrt{1+\frac{2\mu}{\hbar^2k_x^2}\mu_0\mathcal{A}\mathcal{H}^H}.$$

Таким образом, коэффициент отражения R равен

$$R=\left(\frac{B}{A}\right)^2=\left(\frac{k_x-k_{2x}}{k_x+k_{2x}}\right)^2$$

Если спины нейтронов ориентированы в противоположном оси z направлении, то в этом случае

$$k_{2x}=k_x\sqrt{1-\frac{2\mu}{\hbar^2k_x^2}\mu_0\vartheta^2},$$

а в остальном результаты будут те же. Так как μ_0 для нейтрона отрицательно, то угол преломления $\varphi 2\uparrow>\varphi>\varphi_{2\uparrow}$ (см. рис. 27).

В случае произвольной ориентации спина нейтронов волновая функция в области $x>0$ будет иметь вид

$$C_\uparrow\begin{pmatrix}1\\0\end{pmatrix}e^{-ik_\uparrow\boldsymbol{r}}+C_\downarrow\begin{pmatrix}0\\1\end{pmatrix}e^{ik_\downarrow\boldsymbol{r}},$$

где $C_\uparrow$ и $C_{\mathrm{Im}\dot{a}th}$ - коэффициенты разложения начального спинового состояния по состояниям $\begin{pmatrix}1\\0\end{pmatrix}$ и $\begin{pmatrix}0\\1\end{pmatrix}$.

Простая оценка показывает, что даже при (???) $\sim10^4$ заметное отражение будет иметь место только для очень медленных (тепловых) нейтронов ($\lambda\sim1\text{Å}$) и при угле падения φ, отличающемся от $\frac{\pi}{2}$ на доли градуса.

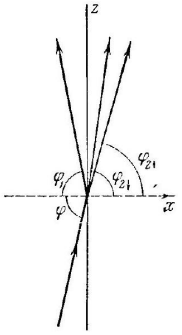


Рис. 27.

ГК-4.17 Вращающееся магнитное поле

Частица со спином 1/2 находится в однородном магнитном поле, постоянном по абсолютной величине и изменяющемся во времени по закону

$$\mathscr{H}_x = \mathscr{H}\sin\vartheta\cos\omega t, \quad \mathscr{H}_y = \mathscr{H}\sin\hat{i}\sin\omega t,$$
$$\mathscr{H}_z = \mathscr{H}\cos\vartheta.$$

В момент времени $t = 0$ проекция спина на направление магнитного поля имела значение $+1/2$. Определить вероятность перехода частицы к моменту времени t в состояние, в котором проекция спина на направление магнитного поля равна - 1/2.

Solution.

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}s_1\\ s_2\end{pmatrix} = -\mu\begin{pmatrix}\mathscr{H}_z & \mathscr{H}_x - i\mathscr{H}_y\\ \mathscr{H}_x + i\mathscr{H}_y & -\mathscr{H}z\end{pmatrix}\begin{pmatrix}s_1\\ s_2\end{pmatrix}$$

$$a := \frac{\mu}{\hbar}\cdot\mathscr{H}\cos\theta, \qquad b := \frac{\mu}{h}\mathscr{H}\sin\theta.$$

$$\frac{ds_1}{dt} = ias_1 + ibe^{-i\omega t}s_2,$$
$$\frac{ds_2}{dt} = ibe^{i\omega t}s_1 ias_2$$

$$s_1 = Ae^{ip_1 t} + Be^{ip_2 t},$$
$$s_2 = e^{i\omega t}\left[\frac{-a+p_1}{b}Ae^{ip_1 t} + \frac{-a+p_2}{b}Be^{ip_2 t}\right],$$

$p_1 := \sqrt{\frac{\omega^2}{4} + a^2 + b^2 + \omega a} - \frac{\omega}{2}, \qquad p_2 := -\sqrt{\frac{\omega^2}{4} + a^2 + b^2 + \omega a} - \frac{\omega}{2}.$

Величины A и B определяются из начальных условий и условия нормировки $|s_1|^2 + |s_2|^2 = 1$.

Проделав несложные вычисления, получаем для вероятности перехода следующие значения:

$$P\left(\frac{1}{2}, -\frac{1}{2}\right) = \frac{\sin^2\vartheta}{1+q^2-2q\cos\theta}\sin^2\left[\frac{t}{2}\omega\left(1-2q\cos\theta+q^2\right)^{1/2}\right]$$

где q есть отношение частоты ларморовской прецессии к частоте вращающегося магнитного поля

$$q := -\frac{2\mu\mathscr{H}}{\hbar\omega} \equiv \frac{\omega_0}{\omega}.$$

Величина q положительна, если магнитное поле вращается в направлении прецессии, и отрицательна, если вращение происходит в обратном направлении.

Если угол θ мал, т. е. $\frac{\sqrt{\mathscr{E}_x^2+\ell_y^2}}{\mathscr{E}_z} \ll 1$, то

$$P\left(\frac{1}{2}, -\frac{1}{2}\right) \approx \frac{\vartheta^2}{(1-q)^2+q\vartheta^2}\sin^2\left[\frac{t}{2}\omega\left[(1-q)^2+q\vartheta^2\right]^{1/2}\right].$$

Из этой формулы следует, что при резонансном соотношении $\omega = \omega_0$, т. е. при $q = +1$ вероятность переориентации магнитного момента относительно магнитного поля, равная $P\left(\frac{1}{2}, -\frac{1}{2}\right) \approx \sin^2\frac{t\omega}{2}\theta$, может оказаться близкой к единице при некотором значении t.

Если же в рассматриваемом случае изменить направление вращения магнитного поля (или изменить знак у $\mathscr{H}_z$), то для вероятности перехода получим величину

$$P\left(\frac{1}{2}, -\frac{1}{2}\right) = \frac{\vartheta^2}{4}\sin^2\omega t$$

значительно меньшую единицы. На основании такого резкого качественного различия можно определить знак магнитного момента частицы

ГК-4.18 (????)

Частица, обладающая спином 1/2 и магнитным моментом μ, движется в неоднородном магнитном поле вида

$$\mathscr{E}\mathscr{H}_z = \mathscr{H}_0 + kz, \quad \mathscr{H}_y = -ky, \quad \mathscr{H}_x = 0 \quad (\mathrm{div}\mathscr{H} = 0).$$

а) Найти выражения для зависящих от времени операторов координат x, y, z.

б) Определить средние значения координат и зависимость дисперсии координат от времени, если волновая функция частицы в момент времени $t = 0$ имеет вид

$$\psi = \varphi(x, y, z)e^{\frac{ip_0 x}{\hbar}}\begin{pmatrix} a \\ p \end{pmatrix}.$$

Solution.

а)

$$\hat{x}(t) = \frac{\hat{p}_x}{m}t + x,$$
$$\hat{y}(t) = -\frac{\mu k}{2m}t^2\hat{\sigma}_y + \frac{\hat{p}_y}{m}t + y,$$
$$\hat{z}(t) = -\frac{\mu k}{2m}t^2\hat{\sigma}_z + \frac{\hat{p}_z}{m}t + z,$$

б)

$$\overline{\bar{z}(t)} = \bar{z}(t) = \frac{\mu k}{2m}t_0^2\hat{\sigma}_z + \frac{\mu k}{2m}t^2\left(\alpha\alpha^* - \beta\beta^*\right),$$
$$\overline{\hat{y}(t)} = (\bar{y})_0 - \frac{\mu k}{2m}t^2\left(i\hat{\beta}^*\alpha - i\beta\alpha^*\right),$$
$$\overline{\hat{x}(t)} = (\bar{x})_0 + \frac{p_0}{m}t,$$

$$\overline{(\Delta\hat{z})_t^2} = \overline{(\Delta z)_0^2} + \frac{\mu^2k^2}{4m^2}t^4\left[1 - (\alpha\alpha^* - \beta\beta^*)^2\right] + \frac{h^2t^2}{m^2}\int\left(\frac{\partial\varphi}{\partial z}\right)^2 d\tau,$$
$$\overline{(\Delta\hat{y})_t^2} = \overline{(\Delta y)_0^2} + \frac{\mu^2k^2}{4m^2}t^4\left[1 - (i\beta^*\alpha - i\beta\alpha^*)^2\right] + \frac{h^2t^2}{m^2}\int\left(\frac{\partial\varphi}{\partial y}\right)^2 d\tau,$$
$$\overline{(\Delta\hat{x})_t^2} = \overline{(\Delta x)_0^2} + \frac{h^2t^2}{m^2}\int\left(\frac{\partial\varphi}{\partial x}\right)^2 d\tau,$$

Замечание. Рассмотрим, например, совокупность частиц, у которых проекция спина на ось z при $t = 0$ с достоверностью имеет значение $+1/2$, т. е. $x = 1, \beta = 0$. Как легко видеть из полученных результатов, если на пути таких частиц, движущихся в неоднородном магнитном поле, поставить экран, то на нем этими частицами будет образовано два пятна. z-координаты этих пятен будут одинаковы, а y-е координаты противоположны по знаку.

ГК-4.19

Нейральная частица находится в пространственно-однородном магнитном поле, изменяющемся во времени лишь по направлению, но не по абсолютной величине.

Написать уравнения для спиновой функции в «ξ» представлении, где ось ξ направлена вдоль магнитного поля. Показать, что в случае достаточно медленного изменения направления магнитного поля вероятности тех или иных значений проекций момента на направление поля не изменяются.

Solution.

(?? если нейтральная, то почему она взаимодействует вообще с МП???)

Направление магнитного поля будем характеризовать полярными углами (?), φ. Углы it и φ являются функциями времени. Оператор Гамильтона для нейтральной частицы представим в виде

$$\hat{H} = -\mu\mathscr{H}?\left(\hat{J}_x\sin\theta\cos\varphi + \hat{J}_y\sin\theta\sin\varphi + \hat{J}_z\cos\theta\right)$$

здесь $\mathscr{H}$ - абсолютное значение напряженности магнитного поля. Обозначим через $\hat{J}_\xi$ оператор момента в направлении магнитного поля

$$\hat{J}_\xi = \hat{J}_x\sin\theta\cos\varphi + \hat{J}_y\sin\vartheta\sin\varphi + \hat{J}_z\cos \geqslant$$

и введем функции $\psi_m(t)$, которые являются собственными функциями оператора $\hat{J}_\xi$, т. е.

$$\hat{J}_\xi \psi_m(t) = m\psi_m(t).$$

Будем искать решение уравнения Шредингера

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$$

В виде

$$\psi = \sum a_m(t)\psi_m(t).$$

Как пізвестно (см. задачу 19§4),

$$\psi_m(t) = e^{-i\hat{J}_z^\varphi \cdot e^{-i\hat{J}_y^\vartheta}}\psi_m^{(0)},$$

где $\psi_m^{(0)}$ удовлетворяет соотношению

$$\hat{J}_z\psi_m^{(0)} = m\psi_m^{(0)}$$

Вычислим сперва $\dot{\psi}_m(t)$. Воспользовавшись соотношениями

$$\begin{aligned}
&e^{i\hat{J}_y^\vartheta}\hat{J}_z e^{-i\hat{J}_y^\vartheta} = \hat{J}_z\cos\geqslant -\hat{J}_x\sin\vartheta,\\
&\hat{J}_{x\psi m}\psi_m^{(0)} = \frac{1}{2}\sqrt{(j+m)(j-m+1)}\psi_{m-1}^{(0)} +\\
&+\frac{1}{2}\sqrt{(j+m+1)(j-m)}\psi_{m+1}^{(0)},\\
&\hat{J}_y''\psi_m^{(0)} = \frac{t}{2}\sqrt{(j+m)(j-m+1)}\psi_{m-1}^{(0)} -\\
&-\frac{i}{2}\sqrt{(j+m+1)(j-m)}\psi_{m+1}^{(0)},
\end{aligned}$$

имеем:

$$\begin{aligned}
\dot{\psi}_m(t) =&(-i\dot{\varphi}m\cos i)\psi_m(t) +\\
&+\frac{1}{2}\sqrt{(\dot{j}+m+1)(j-m)}(\dot{i}\varphi\sin i - \dot{i})\psi_{m+1}(t) +\\
&+\frac{1}{2}\sqrt{(j+m)(j-m+1)}(i\varphi\sin\vartheta + \dot{v})\psi_{m-1}(t).
\end{aligned}$$

Подставляя значение $\dot{\psi}_m(t)$ в выражение

$$i\hbar\sum_m\left\{\psi_m(t)\dot{a}_m(t) + a_m(t)\dot{\psi}_m(t)\right\} = -\mu\mathscr{H}\sum_m ma_m(t)\psi_m(t),$$

получаем систему уравнений, определяющих изменение коэффициентов a_m во времени:

$$\begin{aligned}
i\hbar\frac{da_m}{dt} + m\mu\mu_i\mathcal{H}a_m = &-m\hbar\dot{\varphi}\cos\vartheta a_m +\\
&+\frac{1}{2}\hbar(\dot{\varphi}\sin\vartheta + i\dot{\vartheta})\sqrt{(j+m)(j-m+1)}a_{m-1} +\\
&+\frac{1}{2}\hbar(\dot{\varphi}\sin\vartheta - i\dot{0})\sqrt{(j-m)(j+m+1)}a_{m+1}
\end{aligned}$$

Если

$$\dot{\varphi} \ll \frac{\mu\mathcal{H}}{\hbar}, \quad \dot{v} \ll \frac{\mu\mathcal{H}}{\hbar},$$

т. е. угловая скорость изменения направления магнитного поля много меньше частоты прецессии, то в приведенной системе уравнений можно пренебречь правой частью и тогда

$$a_m \sim e^{i\frac{m\mu\cdot\mathscr{F}}{\hbar}t}$$

Таким образом, в этом случае вероятности различных значений проекции момента на изменяющееся во времени направление магнитного поля остаются постоянными.

ФР.?? Проекция спина (????)

Частица со спином 1/2 находится в однородном магнитном поле, направленном по оси z, изменяющемся по абсолютной величине по произвольному закону $\mathscr{H} = \mathscr{H}(t)$. В начальный момент времени ($t = 0$) спиновая функция имела вид $\begin{pmatrix} e^{-i\alpha}\cos\delta \\ e^{i\alpha}\sin\delta \end{pmatrix}$. Определить среднее значение проекции спина на оси x и y, а также на направление, вдоль которого проекция спина имеет определенное значение в момент времени t.

Solution.

$$i\hbar\frac{\partial s_1}{\partial t} = -\mu_0\mathscr{H}(t)s_1,$$
$$i\hbar\frac{\partial s_2}{\partial t} = \mu_0\mathscr{H}(t)s_2.$$

Решения этих уравнений имеют вид

$$s_1 = c_1 e^{\frac{i\mu_0}{\hbar}\int\limits_0^t \mathscr{H}(t)dt},$$
$$s_2 = c_2 e^{-\frac{ix_1}{\hbar}\int\limits_0^t \mathscr{H}(t)dt}$$

Постоянные c_1 и c_2 находим из начальных условий: $c_1 = e^{-i\alpha}\cos\delta, c_2 = e^{i\alpha}\sin\delta$. Из вида функции s_1 и s_2 следует, что вероятность той или иной ориентации спина на ось z не меняется со временем. Среднее значение проекции спина на ось x определяется выражением

$$\bar{\hat{s}}_x = \frac{\hbar}{2}\sin 2\delta\cdot\cos\left\{\frac{2\mu\mu_0}{\hbar}\int\limits_0^t \mathscr{H}(t)dt - 2x\right\}$$

и аналогично этому

$$\overline{\hat{s}_y} = -\frac{\hbar}{2}\sin 2\hat{\partial}\cdot\sin\left\{\frac{2\mu_0}{\hbar}\int\limits_0^t \mathscr{Z}t(t)dt - 2\alpha\right\}.$$

Направление, вдоль которого проекция спина имеет значение $+1/2$, характеризуется полярными координатами $\Theta = 2\hat{,}$, $\Phi = 2\left(\alpha - \frac{\mu_0}{\hbar}\int\limits_0^t \mathscr{H}(t)dt\right)$. Таким образом, это направление описывает с течением времени коническую поверхность. При постоянной напряженности поля прямая, «вдоль которой направлен спин», равномерно вращается вокруг направления магнитного поля с частотой $\frac{2\mu 0\mathscr{A}}{h}$.

17.3 Basic Scatterings

17.3.1 Problems about Passing though a Barrier 1

(задачник Гольдмана Кривченкова, Галицкого 1981, мощные)
(!!!! самое главное - раздел про взятие интегралов для вкб!!! все в это упирается!!! также условия применимости важно выделить!)

Б-2.2.13 Типичные прохождения (!?!?)

Найти коэффициенты прохождения и отражения:
а) для прямоугольной ямы;
б) для прямоугольного потенциального барьера (рассмотреть случаи, когда энергия падающей частицы больше и меньше высоты потенциального барьера).

Solution. а), для ямы

Как всегда: пишем анзацы, сшиваем, получаем коэффициенты, по ним считаем поток, а от потоков - требуемые коэффициенты.

$$U(x) = \begin{cases} -U_0, & |x| < a/2 \\ 0, & |x| > a/2 \end{cases}$$

$$\psi(x) = \begin{cases} e^{ikx} + Ae^{-ikx}, & x < -a/2, \\ Ce^{ik_1 x} + De^{-ik_1 x}, & |x| < a/2, \\ Be^{ikx}, & x > a/2, \end{cases}$$

$$k^2 := \frac{2mE}{\hbar^2} > 0, \quad k_1^2 := \frac{2m\left(E + U_0\right)}{\hbar^2}.$$

Учет условии непрерывности волновой функции ψ и ее производной ψ' в точках $x = \pm a/2$ дает систему из четырех уравнений.

(?? проделаю, по идее всё решит без проблем)

В результате решения этой системы имеем

$$A = \frac{ie^{-ika}\left(k_1^2 - k^2\right)\sin k_1 a}{2kk_1 \cos k_1 a - i\left(k_1^2 + k^2\right)\sin k_1 a},$$

$$B = \frac{2kk_1 e^{-ik_1 a}}{2kk_1 \cos k_1 a - i\left(k_1^2 + k^2\right)\sin k_1 a}.$$

Reflection:

$$R = \frac{|j_x^{\text{refl}}|}{|j_x^{\text{in}}|} = |A|^2 = \frac{\left(k_1^2 - k^2\right)\sin^2 k_1 a}{4k_1^2 k^2 \cos^2 k_1 a + \left(k_1^2 + k^2\right)^2 \sin^2 k_1 a} = \frac{\left(k_1^2 - k^2\right)\sin^2 k_1 a}{4k_1^2 k^2 + \left(k_1^2 - k^2\right)^2 \sin^2 k_1 a}.$$

$R = 0$ при $k_1 a = \frac{a}{\hbar}\sqrt{2m\left(E + U_0\right)} = n\pi, n = 1, 2, ...$, а также, естественно, при $k = k_1, (U_0 = 0)$.

Transmission:

$$D = \frac{|j_x^{\text{прош}}|}{|j_x^{\text{nan}}|} = |B|^2 = \frac{4k_1^2 k^2}{4k_1^2 k^2 \cos^2 k_1 a + \left(k_1^2 + k^2\right)^2 \sin^2 k_1 a} = \frac{4k_1^2 k^2}{4k_1^2 k^2 + \left(k_1^2 - k^2\right)^2 \sin^2 k_1 a}.$$

Также выполняется $D + R = 1$.

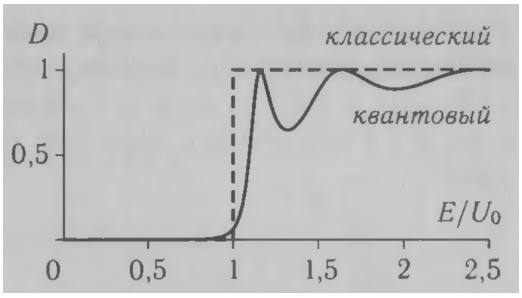
Solution. б), для барьера

Полученные результаты для коэффициентов прохождения и отражения будут справедливы и в случае потенциального барьера

$$U(x) = \begin{cases} 0, & |x| > a/2, \\ U_0, & |x| < a/2, \end{cases}$$

если в формуле $k_1^2 = \frac{2m}{\hbar^2}\left(E + U_0\right)$ осуществить замену $U_0 \to -U_0$. При $0 < E < U_0$ нужно дополнительно положить $k_1 = i\varkappa_1$, где $\varkappa_1^2 = \frac{2m}{\hbar^2}\left(U_0 - E\right)$. В результате получаем

$$R = \frac{\left(\varkappa^2 + k^2\right)\operatorname{sh}^2 \varkappa_1 a}{4\varkappa_1^2 k^2 + \left(\varkappa_1^2 + k^2\right)^2 \operatorname{sh}^2 \varkappa_1 a}, \qquad D = \frac{4\varkappa_1^2 k^2}{4\varkappa_1^2 k^2 + \left(\varkappa_1^2 + k^2\right)^2 \operatorname{sh}^2 \varkappa_1 a}$$



Из рис. видно, что коэффициент прохождения D в квантовом случае достигает максимального значения $D = 1$ (классический предел) лишь при $k_1 a = \pi n, n = 1, 2, ...$ Между этими максимумами находятся минимумы, причем значение D в этих точках растет с ростом величины E/U_0.

Б-2.2.16 Отражение от ямы и стенки

Найти фазу отраженной волны $e^{ikx+i\varphi}$ относительно падающей из бесконечности $-e^{-ikx}$ от потенциала

$$U(x)=\begin{cases}\infty, & x<0\\ -U_0, & 0<x<a\\ 0, & x>a\end{cases}$$

при $|\varepsilon|\ll\hbar^2/\left(2ma^2\right)$. Выразить ее через энергию слабосвязанного уровня ($ka\ll 1$).

Solution.

В соответствии с условием (см. также задачу 2.2.4) выбираем решение в виде

$$\psi(x)=\begin{cases}A\sin k_1x, & 0<x<a,\\ -e^{-ikx}+e^{ikx+i\varphi}=e^{i\varphi/2}2i\sin(kx+\varphi/2), & x\geqslant a.\end{cases}$$

Здесь введены стандартные обозначения:

$$E=\frac{\hbar^2k^2}{2m},\quad U_0=\frac{\hbar^2k_0^2}{2m},\quad k^2+k_0^2=k_1^2.$$

Решение в области $0<x<a$ следует из граничного условия $\psi(0)=0$; φ - дополнительная фаза, приобретенная отраженной волной.

Условие непрерывности логарифмической производной при $x=a$ дает, что

$$ka\operatorname{ctg}(ka+\varphi/2)=k_1a\operatorname{ctg}k_1a.$$

По условию задачи в яме должен быть один слабосвязанный уровень. При глубине ямы

$$U_{0\min}=\frac{\pi^2\hbar^2}{8ma^2}$$

в ней появляется первый дискретный уровень энергии (см. задачу 2.2.4), но его энергия $|\varepsilon|=0$. Поэтому предположим, что глубина ямы $U_0=U_{0\min}(1+\Delta)$, где $\Delta\ll 1$. Раскладывая (2) в предположении $\Delta\ll 1$ и $ka\ll 1$ (омедленные» частицы), получаем условие для определения фазы:

$$\operatorname{ctg}\frac{\varphi}{2}\simeq-\frac{\pi^2\Delta}{8ka}.$$

Величину Δ можно связать с энергией ε слабосвязанного уровня. Для этого в уравнении, определяющем связанные уровни энергии,

$$\operatorname{ctg}Ka=-\frac{\varkappa}{K},\qquad \text{где } |\varepsilon|=\frac{\hbar^2\varkappa^2}{2m}, K^2=k_0^2-\varkappa^2$$

проведем разложение, считая, что $\ll 1, \Delta\ll 1$ (k_0 связано с U_0 обычным соотношением (1)). В результате найдем

$$\varkappa\simeq\frac{\pi^2\Delta}{8a},$$

поэтому окончательно

$$\operatorname{ctg}\frac{\varphi}{2}\simeq-\frac{\varkappa}{k}=-\sqrt{\frac{|\varepsilon|}{E}}.$$

Г.1981-9.26. Сглаженный барьер

Вычислить в квазиклассическом приближении коэффициент прозрачности параболического барьера вида

$$U(x)=\begin{cases}U_0\left(1-x^2/a^2\right), & |x|<a\\ 0, & |x|>a\end{cases}$$

(при этом специально обсудить случай медленных частиц $E\to\to 0$).

Solution.

Г.1981-9.27 Линейный барьер

Оценить в квазиклассическом приближении коэффициент прозрачности барьера вида

$$U(x) = \begin{cases} 0, & x < 0 \\ U_0(1 - x/a), & x > 0 \end{cases}$$

Какова точность полученного результата (сравнить с 9.31 и 9.32)?

Solution.

Стандартная формула для коэффициента прозрачности барьера в квазиклассическом приближении

$$D \approx \exp\left[-\frac{2}{\hbar}\int\limits_{x_1}^{x_1} |p|dx\right] = \exp\left[-\frac{2}{\hbar}\int\limits_{0}^{x_0} \sqrt{2m\,(U_0 - E - U_0 x/a)}dx\right]$$

в рассматриваемой задаче непосредственно не применима, так как в окрестности левой точки поворота $x = 0$ нарушаются условия сшивания квазиклассических решений, использованные при выводе (1) (эти условия приведены в решении предыдущей задачи). Тем не менее формулу (1) можно использовать для оценки коэффициента прозрачности. Элементарное интегрирование дает

$$D \sim \exp\left[-\frac{4a\sqrt{2m}}{3U_0\hbar}\,(U_0 - E)^{3/2}\right].$$

Выражение (2) определяет коэффициент прозрачности лишь по порядку величины (или, как говорят, с точностью до предэкспоненциального множителя, который при $E \sim U_0$ имеет величину порядка единицы; следует, однако, иметь в виду, что при $E \to 0$ этот множитель обращается в нуль -см. 9.32). Однако в случае, когда под знаком экспоненты в этом выражении стоит большое по величине отрицательное число, формула (2) правильно передает основное - экспоненциальную малость коэффициента прозрачности.

Г.1981-9.28.

То же, что и в предыдущей задаче, для барьера вида

$$U(x) = \begin{cases} 0, & x < 0 \\ U_0 \exp(-x/a), & x > 0 \end{cases}$$

(см. также 9.31).

Solution.

Согласно формуле для коэффициента прозрачности барьера в результате элементарного интегрирования находим

$$D \sim \exp\left[\frac{2}{\hbar}\int\limits_{x_1}^{x_2} |p|dx\right] = \exp\left\{-\frac{4a}{\hbar}\sqrt{2mE}\left[\sqrt{\frac{U_0}{E} - 1} - \operatorname{arctg}\sqrt{\frac{U_0}{E} - 1}\right]\right\}.$$

Г.1981-9.30. Гауссов барьер

В квазиклассическом приближении найти коэффициент прозрачности барьера

$$U(x) = \frac{U_0 a^2}{x^2 + a^2}$$

при достаточно малой энергии частиц.

Solution.

9.30. Интеграл в показателе экспоненты в выражении для $D(E)$ заменой переменной $x = a\ \mathrm{sh}\ t$ приводится к виду $\left(\mathrm{sh}\, t_0 = \sqrt{U_0/E - 1} \equiv b^{-1}\right)$

$$\int_{x_1}^{x_2} |p| dx = 2a\sqrt{2m\,(U_0 - E)} \int_0^{t_0} \sqrt{1 - \frac{E}{U_0 - E}\,\mathrm{sh}^2\, t} dt.$$

Инчеграл в выражении (1) представляет собой эллиптический китеграл второго рода. При $E \ll U_0$ этот интеграл легко вычислить приближенно, если учесть, что при этом подкоренное 376 выражение равно единице во всем интервале интегрирования, за исключением узкой области вблизи верхнего иредела интегрирования, в которой $\mathrm{sh}\, t \gg 1$, и поэтому можно положить $\mathrm{sh}^2\, t \approx e^{2t}/4$ (иричем во всем интервале интегрирования!), так что интеграл принимает вид

$$\int_0^t \sqrt{1 - b^2\,\mathrm{sh}^2\, t} dt \approx \int_0^t \sqrt{1 - \frac{b^2}{4} e^{2t}} dt$$

С помощыю замены переменной $(b/2)e^t = \sin z$ интеграл (2) легко вычнсляется и оказывается равным $(b \ll 1)$

$$-1 + \ln\left[4\sqrt{U_0/E}\right].$$

Таким образом,

$$D(E) \approx (E/16U_0)^{\frac{2}{\hbar}}\, a\sqrt{2mU} \cdot \exp\left(\frac{4}{\hbar} a\sqrt{2mU_0}\right).$$

Условиями применимости полученного результата являются

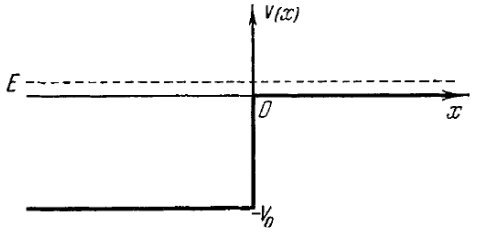
$$\frac{a}{\hbar}\sqrt{2snU_0} \gg 1, \quad E \ll \frac{n}{a}\sqrt{\frac{U_0}{m}},$$

первое из которых обеспечивает применимость квазиклассики. Второе из условий (5) заменяет условие $E \ll U_0$, использованное при вычислении интеграла в выраженни (1). Причина этой замены состоіт в том, что ири приближенном расчете величины f вида $f = e^A$, когда приближеншо вычнсляется значение A, для того чтобы было выполнено условне $f_{\text{точн}}\,/f_{\text{прибл}} \approx 1$, требуется $|A_{\text{точн}} - A_{\text{прибл}}| \ll 1$ (а не просто $A_{\text{точн}}\,/A_{\text{прибл}} \approx 1$, и это обстоятельство следует учитывать в случае $|A| \gg 1$). Внимательный читатель легко убедится в том, что именно второе из условий (5) (а не условие $E \ll U_0$) обеспечивает справедливость полученного значения коэффициента прозрачности.

17.3.2 Problems about Passing though a Barrier 2

ГК-2.1. Отражение электрона от поверхности металла (!?)

При изучении эмиссии электронов металлами необходимо принять во внимание то обстоятельство, что электроны с энергией, достаточной для выхода из металла, согласно квантовой механике, могут отражаться от границы металла. Рассматривая одномерную модель с потенциалом $V = -V_0$ при $x < 0$ (внутри металла) и $V = 0$ при $x > 0$ (вне металла), определить коэффициент отражения электрона с энергией $E > 0$ от поверхности металла.



Solution.

В области металла ($x < 0$) общий вид волновой функции принадлежащей собственному значению E, следующий:

$$\psi_1 = be^{i\varkappa x} + ce^{-i\varkappa x}, \qquad \chi = \frac{\sqrt{2\mu\,(E+V_0)}}{\hbar}.$$

В области $x > 0$ собственная функция имеет вид волны, бегущей из металла

$$\psi_{\mathrm{II}} = ae^{ikx}, \quad \text{где} \quad k = \frac{\sqrt{2\mu E}}{\hbar}.$$

На границе металла волновые функции ψ_{I} и ψ_{II} и их производные должны удовлетворять условию непрерывности

$$\psi_{\mathrm{II}}(0) = \psi_{\mathrm{I}}(0), \quad a = b + c$$
$$\psi'_{\mathrm{II}}(0) = \psi'_{\mathrm{I}}(0), \quad ak = (b - c)\varkappa$$

Отношение плотности потока отраженной волны к плотности потока падающей дает коэффициент отражения

$$R_0 = \left(\frac{\varkappa - k}{\varkappa + k}\right)^2 = \left(\frac{\sqrt{E+V_0} - \sqrt{E}}{\sqrt{E+V_0} + \sqrt{E}}\right)^2 = \frac{V_0^2}{\left(\sqrt{E+V_0} + \sqrt{E}\right)^4}.$$

Если энергия электрона $E = 0$, коэффициент отражения $R_0 = 1$ с возрастанием энергии R_0 быстро уменьшается; при $E \gg V_0$

$$R_0 \approx \frac{V_0^2}{16E^2}.$$

В другом предельном случае $E \ll V_0$

$$R_0 \approx 1 - 4\sqrt{\frac{E}{V_0}}.$$

Для нормальных металлов $V_0 \sim 10$ эв. При этом коэффициент отражения для электронов с энергией $E = 0,1$ эв

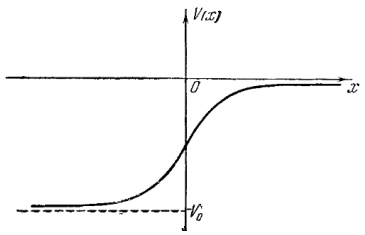
$$R_0 = 0,67.$$

ГК-2.2 Отражение от металла при смытой границе (!?)

В предыдущей задаче предполагалось, что потенциал на границе металла изменяется скачкообразно. В действительности это изменение потенциала прэисходит непрерывно в области, размеры которой порядка междуатомных расстояний в металле. Аппроксимируя потенциал вблизи псверхности металла, с помощью функции

$$V = -\frac{V_0}{e^{\frac{x}{a}} + 1}$$

определить коэффициент отражения электрона с энергией $E > 0$.



Solution.

2. В уравнении Шредингера

$$-\frac{\hbar^2}{2\mu}\psi'' - \left(E + \frac{V_0}{e^{\frac{x}{a}} + 1}\right)\psi = 0$$

произведем подстановку

$$\xi := -e^{-\frac{x}{a}}, \quad \psi := \xi^{-ika}u(\xi), \qquad k := \frac{\sqrt{2\mu E}}{\hbar}.$$

Для функции $u(\xi)$ получим гипергеометрическое уравнение

$$\xi(1-\xi)u'' + (1-2ika)(1-\xi)u' - x_0^2 a^2 u = 0 \quad \left(\varkappa_0 = \frac{\sqrt{2\mu V_0}}{\hbar}\right).$$

Решение уравнения (1), которое при $x \to \infty(\xi \to 0)$ является конечным и асимптотически представляет бегущую волну ce^{ikx}, имеет вид

$$\psi = ce^{ikx} F\left\{i(x-k)a, -i(\varkappa+k)a, 1-2ika, -e^{-\frac{x}{a}}\right\}$$
$$\varkappa := \frac{\sqrt{2\mu\left(E+V_n\right)}}{\hbar}$$

Для того чтобы найти коэффициент отражения, необходимо определить вид волновой функции внутри металла ($x \to -\infty$):

$$\psi \approx c\frac{\Gamma(1-2ika)\Gamma(-2ika)}{\Gamma(-l(x+k)a)\Gamma(1-l(k+\%)a)}e^{i\varkappa x} + c\frac{\Gamma(1-2ika)\Gamma(2ika)}{\Gamma(i(x-k)a)\Gamma(1+i(x-k)a)}e^{-i\varkappa x}.$$

Отсюда находим коэффициент отражения

$$R_a = \left|\frac{\Gamma(2ika)\Gamma(-l(x+k)a)\Gamma(1-i(x+k)a)}{\Gamma'(-2ika)\Gamma^{\top}(i(x-k)a)\Gamma(1+l(x-k)a)}\right|^2 = \frac{\mathrm{sh}^2\,\pi a(\varkappa-k)}{\mathrm{sh}^2\,\pi a(\varkappa+k)}.$$

При вычислении R_a надо воспользоваться соотношениями $\Gamma(z+1) = z\Gamma(z)\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin\pi z}, \Gamma^*(ix) = \Gamma(-ix)$ при действительном x.

При $a \to 0$ формула для коэффициента отражения переходит в выражение для R_0 в случае прямоугольной потенциальной стенки (см. предыдущую задачу).

Легко убедиться, что имеет место неравенство $R_a < R_0$, т. е. коэффициент отражения в случае плавного изменения потенциала меньше, чем в случае скачкообразного изменения. Для $a = 1\text{Å}, V_0 = 10_B, E = 0,1\text{эВ}$ находим $R_a = 0,235$.

ГК-2.3. Отражение от прямоугольного барьера

Определить коэффициент прохождения частицы через прямоугольный барьер (см. рис. 8 (????)).

Solution.

Рассмотрим поток частиц с энергией $E < V_0$, движущихся слева направо. В области III волновая функция представляет собой прошедшую волну

$$\psi_{\text{III}} = Ce^{ikx}, \quad k = \frac{\sqrt{2\mu E}}{\hbar}.$$

В области I имеется как падающая, так и отраженная волны

$$\psi_I = e^{ikx} + Ae^{-ikx}.$$

В области II общее решение уравнения Шредингера

$$-\frac{\hbar^2}{2\mu}\psi''_{\text{II}} - (E-V_0)\,\psi_{\text{II}} = 0$$

имеет вид

$$\psi_{II} = B_1 e^{\alpha x} + B_2 e^{-xx}, \quad x = \frac{\sqrt{2\mu\left(V_0-E\right)}}{\hbar}.$$

Коэффициенты A, B_1, B_2, C определяются из условий непрерывности волновой функции и ее первой производной.

В точке $x = 0$ эти условия приводят к соотношениям:

$$1 + A = B_1 + B_2$$
$$ik(1-A) = x\left(B_1 - B_2\right).$$

Соответственно в точке $x = a$ имеем:

$$B_1 e^{\times a} + B_2 e^{-xa} = Ce^{ika},$$
$$\times \left(B_1 e^{\times a} - B_2 e^{-xa}\right) = ikCe^{ika}.$$

Из этих уравнений находим: $A = C\frac{k^2+\chi^2}{4lk\pi}e^{ika}\left(e^{\chi a} - e^{-\chi a}\right) = C\frac{2\mu V_0}{\hbar^2}\frac{e^{\chi a}-e^{-\chi a}}{4lk\kappa}e^{ika}$, $B_1 = C\cdot\frac{1}{2}\left(1+\frac{ik}{x}\right)e^{ika-xa}$, $B_2 = C\cdot\frac{1}{2}\left(1-\frac{lk}{x}\right)e^{ika+xa}$, $C = -\frac{4lk}{\%}\frac{e^{-ika}}{e^{\chi a}\left(1-\frac{ik}{\chi}\right)^2 - e^{-xa}\left(1+\frac{ik}{\psi}\right)^2}$. Поскольку принятое выражение для падающей волны в ЧИ имело вид e^{ikx}, коэффициент прохождения

$$D = CC^*.$$

Вычисление дает:

$$D = \frac{4k^2x^2}{\left(k^2+x^2\right)^2 \operatorname{sh}^2 xa + 4k^2x^2}.$$

Отметим, что коэффициент прохождения стремится к нулю при переходе к классической механике, т. е. при $\hbar \to 0$. Если $xa \gg 1$ (т. е. $(V_0 - E) \gg \frac{\hbar^2}{2\mu a^2}$), то выражение для коэффициента прохождения принимает более простой вид

$$D \approx 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-\frac{2\sqrt{2\mu(V_0-E)}}{\hbar}a}.$$

Рассмотрим два конкретных примера: а) Электрон с $E = 1$ эз проходит через потенциальный барьер $V_0 = 2$ яв и $a = 1$ ÅA. Для D получаем значение 0,777. б) Пусть теперь на тот же потенциальный барьер падает протон с той же энергией. В этом случае оказывается, что коэффициент прохождения делается исчезающе малым $D = 3,6 \cdot 10^{-19}$.

ГК-2.4. Отражение от прямоугольного потенциального барьера (?)

Определить коэффициент отражения частицы от прямоугольного барьера в случае $E > V_0$ (надбарьерное отражение).

Solution.

(??? неужели еще не прорешал её???)
4.

$$R = \frac{\left(k^2-\gamma^2\right)\sin^2\gamma a}{4k^2\mu^2 + \left(k^2-\gamma^2\right)\sin^2\gamma a} \quad \left(k = \frac{\sqrt{2\mu E}}{\hbar}, \quad x = \frac{\sqrt{2\mu\left(E-V_0\right)}}{\hbar}\right).$$

ГК-2.5. Коэффициент прохождения через $V(x) = \frac{V_0}{\operatorname{ch}^2\frac{x}{a}}$

Вычислить коэффициент прохождения через потенциальный барьер $V(x) = \frac{V_0}{\operatorname{ch}^2\frac{x}{a}}$ (рис. 9) потока частиц, движущихся с энергией $E < V_0$.

Первое решене (?)

5. Для случая $E < V_0$ волновая функция может быть получена из выражения для волновых функций задачи 11 §1 изменением знака у E и V_0.
Общий вид волновой функции, относящейся к энергии E

$$\psi = c_1\left(\operatorname{ch}\frac{x}{a}\right)^{-2\lambda} F\left(-\lambda+\frac{lka}{2}, -\lambda-\frac{ika}{2}, \frac{1}{2}; -\operatorname{sh}^2\frac{x}{a}\right) + c_2\left(\operatorname{ch}\frac{x}{a}\right)^{-2\lambda}\operatorname{sh}\frac{x}{a}F\left(-\lambda+\frac{lka}{2}+\frac{1}{2}, -\lambda+\frac{tka}{2}+\frac{1}{2}, \frac{3}{2}; -\operatorname{sh}^2\frac{x}{a}\right),$$

где

$$\lambda = \frac{1}{4}\left(\sqrt{1-\frac{8\mu V_0 a^2}{\hbar^2}} - 1\right), \quad k = \frac{\sqrt{2\mu E}}{\hbar}.$$

Коэффициенты c_1 и c_2 определяются из того условия, что при $x \to +\infty$ волновая функция имеет асимптотический вид $\psi \sim e^{ikx}$.

Для нахождения асимптотического вида (1) воспользуемся соотношением

$$F(\alpha,\beta,\gamma;z)=\frac{\Gamma(\gamma)\Gamma(\beta-\alpha)}{\Gamma(\beta)\Gamma(\gamma-1)}(-z)^{-\alpha}F\left(\alpha,\alpha+1-\gamma,\alpha+1-\beta;\frac{1}{z}\right)+ \\ +\frac{\Gamma(\gamma)\Gamma(\alpha-\beta)}{\Gamma(\alpha)\Gamma(\gamma-\beta)}(-z)^{-\beta}F\left(\beta,\beta+1-\gamma,\beta-1-\alpha;\frac{1}{z}\right).$$

Отсюда находим:

$$\psi_{x\to-\infty}\sim(-1)^{2\lambda}\left\{(c_1A_1-c_2A_2)\left(-\frac{1}{2}\right)^{-ika}e^{ikx}+(c_1B_1-c_2B_2)\left(-\frac{1}{2}\right)^{ika}e^{-ikx}\right\}$$
$$\psi_{x\to+\infty}\sim\left\{(c_1A_1+c_2A_2)\left(\frac{1}{2}\right)^{-ika}e^{-ikx}+(c_1B_1+c_2B_2)\left(\frac{1}{2}\right)^{ika}e^{kx}\right\}$$

где для удобства введены обозначения

$$A_1=\frac{\Gamma\left(\frac{1}{2}\right)\Gamma(-ika)}{\Gamma\left(-\lambda-\frac{ika}{2}\right)\Gamma\left(\lambda+\frac{1}{2}-\frac{ika}{2}\right)},$$
$$A_2=\frac{\Gamma\left(\frac{3}{2}\right)\Gamma(-ika)}{\Gamma\left(-\lambda+\frac{1}{2}-\frac{ika}{2}\right)\Gamma\left(\lambda+1-\frac{ika}{2}\right)},$$
$$B_1=\frac{\Gamma\left(\frac{1}{2}\right)\Gamma(ika)}{\Gamma\left(-\lambda+\frac{ika}{2}\right)\Gamma\left(\lambda+\frac{1}{2}+\frac{ika}{2}\right)},$$
$$B_2=\frac{\Gamma\left(\frac{3}{2}\right)\Gamma(ika)}{\Gamma\left(-\lambda+\frac{1}{2}+ika\right)\Gamma\left(\lambda+1+\frac{ika}{2}\right)}.$$

Различие в знаке перед коэффициентом c_2 в выражениях (2) и (3) объясняется тем, что $\operatorname{sh}\frac{x}{a}$ функция нечетная и второй член выражения (1) меняет знак при переходе от положительных к отрицательным значениям x.

Требование того, чтобы на $+\infty$ была только прошедшая волна, приводит к следующей связи коэффициентов c_1 и c_2:

$$c_1A_1+c_2A_2=0.$$

При этом коэффициент прохождения будет иметь вид

$$D=\frac{|c_1B_1+c_2B_2|^2}{|c_1A_1-c_2A_2|^2}.$$

Подставляя в последнее выражение значения коэффициентов A_1,A_2,B_1,B_2 и производя несложные преобразования, получим окончательно:

$$D=\frac{\operatorname{sh}^2\pi ka}{\operatorname{sh}^2\pi ka+\cos^2\left(\frac{\pi}{2}\sqrt{1-\frac{8\mu V_0a^2}{\hbar^2}}\right)},\quad\text{если }\frac{8\mu V_0a^2}{\hbar^2}<1$$

$$D=\frac{\operatorname{sh}^2\pi ka}{\operatorname{sh}^2\pi ka+\operatorname{ch}^2\left(\frac{\pi}{2}\sqrt{\frac{8\mu V_0a^2}{\hbar^2}-1}\right)},\quad\text{если }\frac{8\mu V_0a^2}{\hbar^2}>1.$$

Второе решение

Также эта задача в Галицкий задачник.1981-9.29. Вычислить в квазиклассическом приближении коэффициент прозрачности барьера

$$U(x)=\frac{U_0}{\operatorname{ch}^2(x/a)}.$$

В выражении

$$D=\exp\left[-\frac{2}{\hbar}\int\limits_{x_1}^{x}|p|dx\right]=\exp\left\{-\frac{2\sqrt{2mE}}{\hbar}\int\limits_{-x_3}^{x_1}\sqrt{\frac{U_0}{E\operatorname{ch}^2(x/a)}-1}dx\right\}$$

интеграл заменой переменной

$$\mathrm{sh}(x/a) = x\sin t_3 \quad x = \sqrt{U_0/E - 1},$$

приводится к виду

$$2ax^2 \int\limits_0^{\pi/2} \frac{\cos^2 t dt}{1 + x^2 \sin^2 t} = \pi a \left(\sqrt{1+x^2} - 1\right) = \pi a \left(\sqrt{\frac{U_0}{E}} - 1\right),$$

и коэффициент прозрачности оказывается равным

$$D(E) \approx \exp\left\{-\frac{2\pi a}{\hbar}\sqrt{2m}\left(\sqrt{U_0} - \sqrt{E}\right)\right\}.$$

Условие применимости выражения (2) предполагает $D \ll 1$ (более точно: требуется, чтобы был велик модуль показателя экспоненты), т. е.

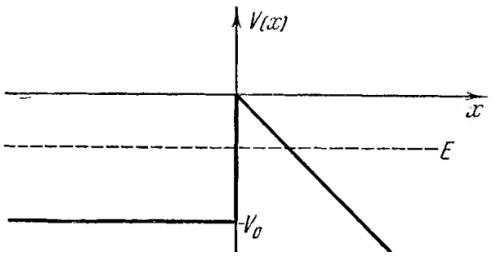
$$\frac{2\pi a}{\hbar}\sqrt{2m}\left(\sqrt{U_0} - \sqrt{E}\right) \gg 1.$$

Кроме этого имеется еще ограничение на энергию частицы E, так как при $E \to 0$ в окрестности точек поворота нарушаются стандартные условия сшивания квазиклассических решений, основанные на линейной аппроксимации потенциала и приводящие к выражению (1) для прозрачности барьера (сравнить с 9.26). Внимательный читатель легко получит, что указанное ограничение имеет вид

$$\sqrt{E} \gg \sqrt{\hbar^2/ma^2}.$$

ГК-2.6. Выход электронов из металла

Вычислить в квазиклассическом приближении коэффициент прохождения электронов через поверхность металла под действием сильного электрического поля напряженности F (рис. нижу). Найти границы применимости расчета.



Solution.

Обычная формула Гамова из квазиклассики решает быстро задачу.

(??? почему если поле есть, то у нас именно так вот меняется потенциал??? это по идее в теории нужно указать.)

Потенциальная энергия электрона имеет вид, изображенный на рис. 10. Коэффициент прохождения

$$D \approx e^{-\frac{2}{\hbar}\int\limits_0^{x_0}\sqrt{2\mu(|E|-Fx)}dx},$$

где точки $x = 0, x = x_0 = \frac{|E|}{F}$ ограничивают область, недоступную частице согласно классической механике. Производя вычисление интеграла в экспоненте, находим:

$$D \approx e^{-\frac{4}{3}\frac{\sqrt{2\mu}}{\hbar F}|E|^{3/2}}.$$

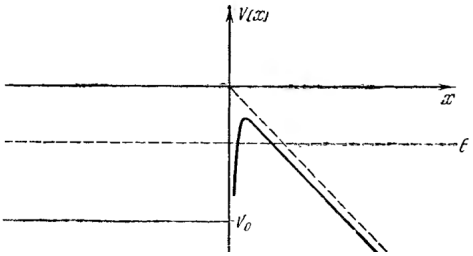
Для выяснений границ применимости этого результата вспомним, что квазиклассическое рассмотрение неприменимо вблизи классической точки поворота x_0 внутри области $x - x_0 \leq \left(\frac{\hbar}{2\mu\cdot F}\right)^{1/3}$. То есть решение применимо в том случае, если область поворота меньше ширины барьера $x_0 = \frac{|E|}{F}$, откуда $\left(\frac{\hbar^2}{2\mu F}\right)^{1/3} \ll \frac{|E|}{F}$ или

$$\frac{\sqrt{2\mu}}{\hbar F}|E|^{3/2} \gg 1.$$

Таким образом, это требование эквивалентно требованию малости коэффициента прохождения $D \ll 1$. Коэффициент прохождения D быстро убывает с ростом $|E|$ и растет с увеличением F.

ГК-2.7. Выход из металла, точнее модель

Рассмотрим модель выхода электронов из металла, в которой изменение потенциала вблизи поверхности происходит непрерывно. Так, например, потенциал электрического изображения $V_{\text{el-im}} = -\frac{e}{4x}$ действует на больших расстояниях от поверхности. Определить коэффициент прохождения D электронов через поверхность металла в электрическом поле с учетом силы электрического изображения (рис. ниже).



Solution..

Используем обычные методы квазиклассики, интеграл сводится к эллиптическому.
(??? что за электрическое изображение тут? буду ЭД смотреть - отвечу про это, пока это просто слова.)
Суммарная потенциальная энергия имеет вид:

$$V = -Fx - \frac{e^2}{4x}.$$

Следует заметить, что это выражение при малых x (порядка атомного расстояния) становится непригодным. Однако для вычисления коэффициента прохождения точный ход потенциала вблизи этой области несущественен. Коэффициент прохождения

$$D \approx \exp\left\{-\frac{2}{\hbar}\int\limits_{x_1}^{x_2}\sqrt{2\mu\left(|E| - Fx - \frac{e^2}{4x}\right)}dx\right\} = \exp\left\{-\frac{2}{\hbar}\int\limits_{x_1}^{x_2} p dx\right\}$$

Причем точки поворота x_1 и x_2 определяются из условия обращения в нуль классического импульса частицы

$$p = \sqrt{2\mu\left(|E| - Fx - \frac{e^3}{4x}\right)} = 0,$$

$$x_{1,2} = \frac{|E| \pm \sqrt{E^4 - e^2F}}{2F}.$$

Тут интеграл

$$\int\limits_{x_1}^{x_2} p dx = \sqrt{2\mu}\int\limits_{x_1}^{x_2}\sqrt{|E| - Fx - \frac{e^2}{4x}}dx$$

представляет собою полный эллиптический интеграл. Заменой независимой переменной $\frac{F}{|E|}x = \xi$ интеграл сводится к функции одного параметра

$$\int\limits_{x_1}^{x_3} p dx = \frac{2}{3}\sqrt{2\mu}\frac{|E|^{3/2}}{F}\varphi(y), y = \frac{\sqrt{e^2F}}{|E|}.$$

Здесь $\varphi(y) := \int\limits_{\xi_1}^{\xi_2}\sqrt{1 - \frac{y^2}{\xi} - \xi}d\xi$, пределы интегрирования ξ_1, ξ_2 определяются из условия обращения в нуль подкоренного выражения. Вводя обозначение $k_0 := \frac{4}{3}\sqrt{2\mu}\frac{|E|^{5/2}}{F}$, получим

$$D = e^{-k_u\varphi(y)}.$$

Отметим, что коэффициент прохождения без учета электрического изображения уже найден ($y = 0$) и равен $D = e^{-k_0}$. Значения $\varphi(y)$ приведены в таблице ниже.

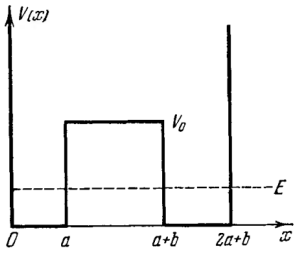
y	0	0,2	0,3	0,4	0,5	0,6	0,7	0,8	0,9	1,0
$\varphi(y)$	1,000	0,951	0,904	0,849	0,781	0,696	0,603	0,494	0,345	0,000

(не нужная таблица на самом деле, но ладно, пусть побудет.)

17.3.3 Problems about Passing though a Barrier 3

ГК-2.8. Колодец с тумбочкой

Определить приближенно уровни энергии и волновые функции частицы в симметричном потенциальном поле вида колодца с тумбочкой (см. рис. ниже), если $E \ll V_0$ и проницаемость барьера мала $\left(\frac{2\mu V_0}{\hbar^2} b^2 \gg 1\right)$.



Solution.

Пишем общий возможный вид волновых функций в трех областях, сшиваем. (все?)
Волновая функция имеет следующий вид:

$$\begin{aligned}
&\psi_{\mathrm{I}} = A\sin kx && 0 < x < a,\\
&\psi_{\mathrm{II}} = B_1 e^{\varkappa} + B_2 e^{-\varkappa x}, && a < x < a+b,\\
&\psi_{\mathrm{III}} = C\sin k(2a+b-x), && a+b < x < 2a+b,
\end{aligned}$$

здесь $k = \frac{\sqrt{2\mu E}}{\hbar}$, $\varkappa = \frac{\sqrt{2\mu(V_0-E)}}{\hbar}$. Условия непрерывности волновой функции и ее произволной приводят к следующим соотношениям:

$$\begin{aligned}
A\sin ka &= B_1 e^{\varkappa a} + B_2 e^{-\varkappa a},\\
Ak\cos ka &= \varkappa\left(B_1 e^{xa} - B_2 e^{-xa}\right),\\
B_1 e^{\varkappa(a+b)} + B_2 e^{-\varkappa(a+b)} &= C\sin ka,\\
\varkappa\left(B_1 e^{\varkappa(a+b)} - B_2 e^{-\varkappa(a+b)}\right) &= -Ck\cos ka.
\end{aligned}$$

Исключая из этих уравнений B_1 и B_2, находим:

$$\begin{aligned}
\left(\frac{\varkappa}{k}\operatorname{tg} ka + 1\right) Ae^{\varkappa b} &= \left(\frac{\varkappa}{k}\operatorname{tg} ka - 1\right) C,\\
\left(\frac{\varkappa}{k}\operatorname{tg} ka - 1\right) Ae^{-\varkappa b} &= \left(\frac{\varkappa}{k}\operatorname{tg} ka + 1\right) C.
\end{aligned}$$

Из условия обращения в нуль детерминанта

$$\begin{vmatrix} \left(\frac{\varkappa}{k}\operatorname{tg} ka + 1\right) e^{\varkappa b} & -\left(\frac{\varkappa}{k}\operatorname{tg} ka - 1\right)\\ \left(\frac{\varkappa}{k}\operatorname{tg} ka - 1\right) e^{-\varkappa b} & -\left(\frac{\varkappa}{k}\operatorname{tg} ka + 1\right) \end{vmatrix} = 0$$

получаем:

$$\left(\frac{\varkappa}{k}\operatorname{tg} ka + 1\right) e^{\varkappa b} = \pm\left(\frac{\varkappa}{k}\operatorname{tg} ka - 1\right).$$

Это уравнение определяет уровни энергии.
Воспользовавшись неравенством

$$xb \gg 1,$$

последнее уравнение можно приближенно представить в следующем виде:

$$\operatorname{tg} ka = -\frac{k}{\varkappa} \mp 2\frac{k}{\varkappa} e^{-\varkappa b}.$$

Правая часть равенства представляет собою малую величину. В нулевом приближении получаем ($k \ll \varkappa$):

$$k_0 = \frac{n\pi}{a}, \quad E_n^{(0)} = \frac{n^2\pi^2\hbar^2}{2\mu a^2}$$

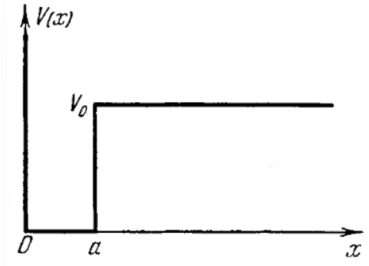
- значения энергии для частицы в потенциальном ящике.

В следующем приближении

$$k = \frac{n\pi}{a} - \frac{k_0}{a\varkappa_0} \mp 2\frac{k_0}{a\varkappa_0} e^{-\varkappa_0 b} \quad (n = 1, 2, 3, ...),$$

$$E_n = E_n^{(0)} - \frac{2E_n^{(0)}}{a\varkappa_0} \mp 4\frac{E_n^{(0)}}{a\varkappa_0} e^{-\varkappa_0 b}, \quad \varkappa_0 = \frac{\sqrt{2\mu\left(V_0 - E_n^{(1)}\right)}}{\hbar}.$$

Первые два члена $E_n^{(1)} = E_n^{(0)} - \frac{2E_n^{(0)}}{a\varkappa_0}$ не зависят от b и дают приближенные значения уровней энергии для частицы в потенциальной яме при $b \to \infty$. См. рис. ниже.



В этом приближении уровни двукратно вырождены; это соответствует возможности нахождения частицы как в области I, так и в области III. Учет конечности b, т. е. возможности прохождения частицы через потенциальный барьер, приводит к расщеплению уровней. Это расщепление экспоненциально мало. Найдем в рассматриваемом приближении коэффициенты A, B_1, B_2 и C. Нижнему уровню

$$E_n^- = E_n^{(1)} - 4\frac{E_n^{(0)}}{a\gamma_0} e^{-\varkappa_0 b}$$

соответствуют

$$B_1 = (-1)^{n-1}\frac{k_0}{\varkappa_0} e^{-\varkappa_0(b+a)} A,$$
$$C = A,$$
$$B_2 = (-1)^{n-1}\frac{k_0}{\varkappa_0} e^{\varkappa_0 a} A.$$

Верхнему уровню

$$E_n^+ = E_n^{(1)} + 4\frac{E_n^{(0)}}{ax_0} e^{-x_v b}$$

соответствуют коэффициенты

$$B_1 = -(-1)^{n-1}\frac{k_0}{\varkappa_0} e^{-\varkappa_0(a+b)} A,$$
$$C = -A,$$
$$B_2 = (-1)^{n-1}\frac{k_0}{\varkappa_0} e^{\varkappa_0 a} A.$$

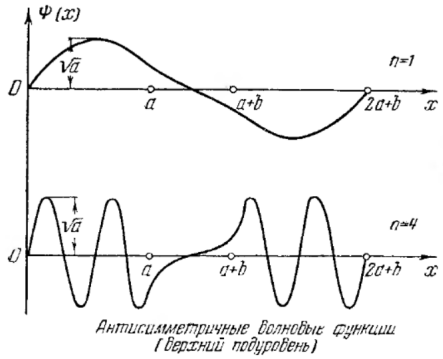
Значение A, определяемое из условия нормировки, равно $\frac{1}{\sqrt{a}}$ (при вычислении нормировочного интеграла долей, вносимой областью II, можно пренебречь).

Таким образом, нижнему уровню соответствует волновая функция

$$\psi_1 = \frac{1}{\sqrt{a}} \sin kx,$$

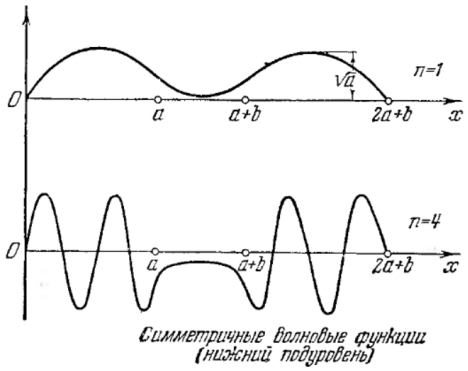
$$\psi_{\text{II}} = (-1)^{n-1}\frac{1}{\sqrt{a}}\frac{k_0}{\varkappa_0}\left\{e^{-\varkappa_0(x-a)} + e^{-\varkappa_0(a+b-x)}\right\},$$

$$\psi_{\text{III}} = \frac{1}{\sqrt{a}} \sin k(2a + b - x).$$



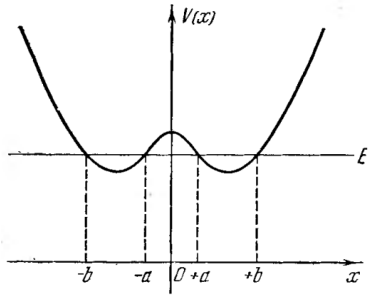
Соответственно для верхнего уровня находим:

$$\psi_{\mathrm{I}} = \frac{1}{\sqrt{a}} \sin kx,$$
$$\psi_{\mathrm{II}} = (-1)^{n-1} \frac{1}{\sqrt{a}} \frac{k_0}{\varkappa_0} \left\{ e^{-\varkappa_0 (x-a)} - e^{-\varkappa_0 (a+b-x)} \right\},$$
$$\psi_{\mathrm{III}} = -\frac{1}{\sqrt{a}} \sin k(2a-b-x).$$



ГК-2.9. Квазиклассика в самбреро (!!!!)

Симметричное поле $V(x)$ представляет собой две потенциальные ямы, разделенные барьером как на рисунке:



Считая выполненным условие квазиклассичности, определить уровни энергии частицы в поле $V(x)$. Сравнить полученный энергетический спектр с энергетическим спектром отдельной ямы. Найти расщепление энергетических уровней отдельной ямы.

Solution.

(?!?!! скоро продумаю, тут типичный метод!)

$$\psi(x<-b)=\frac{c}{\sqrt{|p|}}e^{-\frac{1}{\hbar}\int\limits_{x}^{-b}|p|dx}$$

$$\psi(-b<x<-a)=\frac{c}{\sqrt{p}}e^{-i\frac{\pi}{4}}e^{\frac{i}{\hbar}\int\limits_{-b}^{x}pdx}+\frac{c}{\sqrt{p}}e^{i\frac{\pi}{4}}e^{-\frac{i}{\hbar}\int\limits_{-b}^{x}pdx}=$$
$$=\frac{c}{\sqrt{p}}e^{-i\frac{\pi}{4}}e^{\frac{i}{\hbar}\int\limits_{-b}^{-a}pdx}e^{-\frac{i}{\hbar}\int\limits_{x}^{-a}pdx}+\frac{c}{\sqrt{p}}e^{i\frac{\pi}{4}}e^{-\frac{i}{\hbar}\int\limits_{-b}^{-a}pdx}e^{\frac{i}{\hbar}\int\limits_{x}^{-a}pdx}.$$

$$\psi(-a<x<+a)=ce^{-i\frac{\pi}{4}}e^{\frac{i}{\hbar}\int\limits_{-b}^{-a}pdx}\left\{\frac{e^{-i\frac{\pi}{4}}}{2\sqrt{|p|}}e^{-\frac{1}{\hbar}\int\limits_{-a}^{x}|p|dx}+\frac{e^{i\frac{\pi}{4}}}{\sqrt{|p|}}e^{\frac{1}{\hbar}\int\limits_{-a}^{x}|p|dx}\right\}+$$
$$+ce^{i\frac{\pi}{4}}e^{-\frac{i}{\hbar}\int\limits_{-b}^{-a}pdx}\left\{\frac{e^{i\frac{\pi}{4}}}{2\sqrt{|p|}}e^{-\frac{1}{\hbar}\int\limits_{-a}^{x}|p|dx}+\frac{e^{-i\frac{\pi}{4}}}{\sqrt{|p|}}e^{\frac{1}{\hbar}\int\limits_{-a}^{x}|p|dx}\right\}=$$

$$=\frac{c}{\sqrt{|p|}}\sin\left(\frac{1}{\hbar}\int\limits_{-b}^{-a}pdx\right)e^{-\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx}e^{\frac{1}{\hbar}\int\limits_{x}^{+a}|p|dx}+\frac{2c}{\sqrt{|p|}}\cos\left(\frac{1}{\hbar}\int\limits_{-b}^{-a}pdx\right)e^{\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx}e^{-\frac{1}{\hbar}\int\limits_{x}^{+a}|p|dx}$$

$$\psi(+a<x<+b)=c\sin\left(\frac{1}{\hbar}\int\limits_{-b}^{-a}pdx\right)e^{-\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx}\left\{\frac{e^{-i\frac{\pi}{4}}}{2\sqrt{p}}e^{-\frac{i}{\hbar}\int\limits_{+a}^{x}pdx}+\frac{e^{i\frac{\pi}{4}}}{2\sqrt{p}}e^{\frac{i}{\hbar}\int\limits_{+a}^{x}pdx}\right\}+$$
$$+2c\cos\left(\frac{1}{\hbar}\int\limits_{-b}^{-a}pdx\right)e^{\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx}\left\{\frac{e^{-i\frac{\pi}{4}}}{\sqrt{p}}e^{\frac{i}{\hbar}\int\limits_{+a}^{x}pdx}+\frac{e^{i\frac{\pi}{4}}}{\sqrt{p}}e^{-\frac{i}{\hbar}\int\limits_{a}^{x}pdx}\right\}=$$

$$=\frac{c}{\sqrt{p}}\left\{\frac{1}{2}\sin\left(\frac{1}{\hbar}\int\limits_{-b}^{-a}pdx\right)e^{-\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx-i\frac{\pi}{4}}+2\cos\left(\frac{1}{\hbar}\int\limits_{-a}^{+a}pdx\right)e^{\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx+i\frac{\pi}{4}}\right\}e^{-\frac{i}{\hbar}\int\limits_{+a}^{+b}pdx}e^{\frac{i}{\hbar}\int\limits_{x}^{b}pdx}+$$
$$+\frac{c}{\sqrt{p}}\left\{\frac{1}{2}\sin\left(\frac{1}{\hbar}\int\limits_{-b}^{-a}pdx\right)e^{-\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx+i\frac{\pi}{4}}+2\cos\left(\frac{1}{\hbar}\int\limits_{-a}^{+a}pdx\right)e^{\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx-i\frac{\pi}{4}}\right\}e^{\frac{i}{\hbar}\int\limits_{+a}^{+b}pdx}e^{-\frac{i}{\hbar}\int\limits_{x}^{+b}pdx}.$$

(????откуда выр ниже?? видимо, общее правило тут какое-то применено, а выше мы явно делали?)

$$\psi(x>+b)=\frac{c}{\sqrt{|p|}}\left\{\frac{1}{2}\sin\left(\frac{1}{\hbar}\int\limits_{a}^{b}pdx\right)\cos\left(\frac{1}{\hbar}\int\limits_{a}^{b}pdx\right)e^{-\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx}+\right.$$
$$\left.+2\cos\left(\frac{1}{\hbar}\int\limits_{a}^{b}pdx\right)\sin\left(\frac{1}{\hbar}\int\limits_{a}^{b}pdx\right)e^{\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx}\right\}e^{-\frac{1}{\hbar}\int\limits_{b}^{x}|p|dx}+$$
$$+\frac{c}{\sqrt{|p|}}\left\{-\sin^2\left(\frac{1}{\hbar}\int\limits_{a}^{b}pdx\right)e^{-\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx}+4\cos^2\left(\frac{1}{\hbar}\int\limits_{a}^{b}pdx\right)e^{\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx}\right\}e^{\frac{1}{\hbar}\int\limits_{b}^{x}|p|dx}.$$

Для того чтобы решение при $x\to+\infty$ стремилось к нулю, необходимо, чтобы коэффициент при $e^{\frac{1}{\hbar}\int\limits_{b}^{x}|p|dx}$ обращался в нуль, т. е.

$$-\sin^2\left(\frac{1}{\hbar}\int\limits_{a}^{b}pdx\right)e^{-\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx}+4\cos^2\left(\frac{1}{\hbar}\int\limits_{a}^{b}pdx\right)e^{\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx}=0$$

$$\operatorname{ctg}\left(\frac{1}{\hbar}\int\limits_a^b p dx\right) = \pm\frac{1}{2}e^{-\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx}.$$

Считая прозрачность барьера малой величиной, получаем условие для определения уровней энергии

$$\frac{1}{\hbar}\int\limits_a^b p dx = \pi\left(n+\frac{1}{2}\right) \pm \frac{1}{2}e^{-\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx}.$$

(??? не совсем понял, откуда такие условия? почему не просто было бы πn?)

Обозначим через $E_n^{(0)}$ уровни энергии отдельной потенциальной ямы

$$\frac{1}{\hbar}\int\limits_a^b \sqrt{2\mu\left(E_n^{(0)}-V\right)}dx = \pi\left(n+\frac{1}{2}\right).$$

Уровни энергии в двойной яме $E_n = E_n^{(0)} + \Delta E_n$ найдем из полученного условия квантования, разлагая $\sqrt{2\mu(E_n - V)}$ в ряд по ΔE_n и ограничиваясь линейным членом по ΔE_n

$$\Delta E_n \frac{\mu}{\hbar}\int\limits_a^b \frac{dx}{\sqrt{2\mu\left(E_n^{(0)}-V\right)}} = \pm\frac{1}{2}e^{-\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx}$$

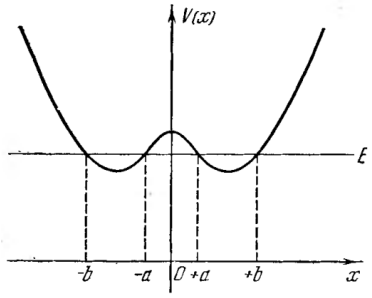
$$\Delta E_n = \pm\frac{\hbar\omega}{2\pi}e^{-\frac{1}{\hbar}\int\limits_{-a}^{+}|p|dx},$$

где ω - циклическая частота классического движения в отдельной яме $\frac{2\pi}{\omega} = 2\mu\int\limits_a^b \frac{dx}{p}$.

Расщепление уровня E_n равно $2|\Delta E_n|$.

ГК-2.10. Переход в самбребо (!?!??!)

Предположим, что до момента времени $t = 0$ между двумя симметричными потенциальными ямами вида



существовала непроницаемая перегородка и частица находилась в левой яме в стационарном состоянии. Определить, по прошествии какого времени τ после удаления перегородки частица окажется в правой яме.

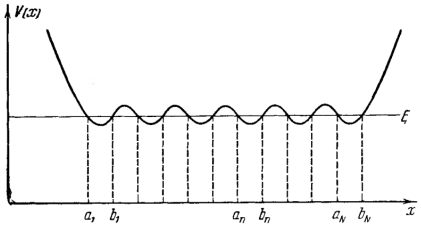
Solution.

(есть только ответ, сам решу потом ее, видимо, решение следует из ответа на пред. задачу)

$$10.\ \tau = -\frac{\pi^2}{\omega}e^{\frac{1}{\hbar}\int\limits_{-a}^{+a}|p|dx},$$

ГК-2.11. Стиральная доска

Поле $V(x)$ представляет собой N одинаковых потенциальных ям, разделенных одинаковыми потенциальными барьерами:



Считая выполненным условие квазиклассичности, определить уровни энергии в поле $V(x)$. Сравнить полученный энергетический спектр с энергетическим спектром отдельной ямы.

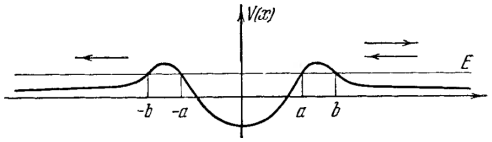
Solution.

Это очень большая задача на страницы 4, когда-то решу.

В области n-го потенциального барьера $b_n < x < < a_{n+1}$ волновую функцию запишем в виде
$\psi = \frac{C_n}{\sqrt{|p|}} e^{-\frac{1}{\hbar}\int_{b_n}^{x}|p|dx} + \frac{D_n}{\sqrt{|p|}} e^{\frac{1}{\hbar}\int_{b_n}^{x}|p|dx} =$
$+\frac{D_n}{\sqrt{|p|}} e^{\frac{1}{\hbar}\int_{b_n}^{a_{n+1}}|p|dx} e^{-\frac{1}{\hbar}\int_{x}^{a_{n+1}}|p|dx};$
продолжая эту функцию в область $(n+1)$-го потенциального барьера $b_{n+1} < x < a_{n+2}$, будем иметь:
(снова формулы на 1 страницу, нет на них сил.)

ГК-2.12. Два холма

Считая выполненными условия квазиклассичности, найти квазистационарные уровни частицы в следующем симметричном поле:



Найти также коэффициент прохождения $D(E)$ для частиц с энергией $E < V_0$.

Solution.

Это очень большая задача на страницы 2, когда-то решу.

ПТФ-12.з1. Отражение методом линий Стокса (40 б).

Найдите с экспоненциальной точностью в рамках квазиклассического приближения вероятность надбарьерного отражения частицы большой энергии E в потенциале $U(x) = -U_0 \frac{x^4}{a^4}$.

1) Идентифицируйте квазиклассические точки остановки; нарисуйте (схематично) линии Стокса и анти-Стокса, соответствующие этой задаче.

2) Выберите любую из интересующих нас линий анти-Стокса, вдоль которых необходимо исследовать решение. Определите условия сшивки амплитуд квазиклассических решений в окрестности необходимых точек остановки. Определите связь амплитуды прохождения и отражения в соответствующей задаче рассеяния.

3) Вычислите необходимые квазиклассические интегралы, найдите ответ.

Solution.

(????)
• Произвольное решение раскладывается по паре линейно независимых:

$$\psi(z) = C_+\psi_+(z) + C_-\psi_-(z)$$

$$\psi_\pm(z) = \frac{1}{\sqrt{p(z)}} e^{\pm iS(z)}, \quad S(z) = \int p(z)dz$$

Идентифицируем точки остановки:

$$p(z_k) = \sqrt{2m\left(E + U_0\frac{z_k^4}{a^4}\right)} = 0$$

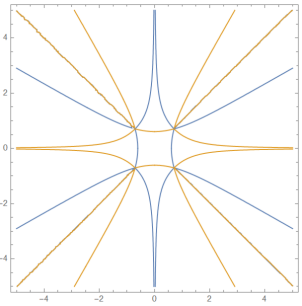
$$z_k = a\sqrt[4]{\frac{E}{U_0}}\exp\left(\frac{i\pi}{4} + \frac{i\pi k}{2}\right), \quad k \in \{0,1,2,3\}$$

$$S(z) = \int\limits_{z_k}^{z} \sqrt{2m\left(E + U_0\frac{z^4}{a^4}\right)}dz$$

Линии Стокса и анти-Стокса задаются соответственно уравнениями:

$$\begin{cases} \mathrm{Re}S(z) = 0, \\ \mathrm{Im}S(z) = 0. \end{cases}$$

Линии Стокса (синие) и анти-Стокса (жёлтые) изображены на рис. ниже



• Задача рассеяния:

$$\psi(x) = \begin{cases} \frac{1}{\sqrt{p(x)}} e^{i\int_0^x p(z)dz} + \frac{r}{\sqrt{p(x)}} e^{-i\int_0^x p(z)dz}, & x < 0 \\ \frac{t}{\sqrt{p(x)}} e^{i\int_0^x p(z)dz}, & x > 0 \end{cases} = \begin{cases} e^{i\int_0^x p(z)dz}\psi_+(x) + re^{-i\int_0^x p(z)dz}\psi_-(x), & \mathrm{Re}\, x < 0 \\ te^{i\int_0^x p(z)dz}\psi_+(x), & \mathrm{Re}\, x > 0 \end{cases}$$

Для нахождения t выберем контур из линий анти-Стокса, приближающихся к действительной оси на бесконечности. При обходе точек остановки дважды пересекается линия Стокса.

Решение между линиями Стокса:

$$\psi(z) = \frac{C'_+}{\sqrt{p(z)}} e^{i\int_{z_0}^z p(z')dz'}$$

Связь между t и C'_+:

$$C'_+ = te^{i\int_0^{z_0} p(z')dz'}$$

Решение после перехода через 2 линию Стокса:

$$\psi(z) = \frac{C''_+}{\sqrt{p(z)}} e^{i\int_{z_1}^z p(z')dz'}$$

Связь между t и C''_+:

$$C''_+ = C'_+ e^{i\int\limits_{z_0}^{z_1} p(z')dz'} = te^{i\int\limits_{0}^{z_0} p(z')dz'} e^{i\int\limits_{z_0}^{z_1} p(z')dz'}$$

Условие сшивки:

$$C''_+ e^{i\int\limits_{z_1}^{0} p(z')dz'} = 1$$

$$te^{i\int\limits_{0}^{z_0} p(z')dz'} e^{i\int\limits_{z_0}^{z_1} p(z')dz'} e^{i\int\limits_{z_1}^{0} p(z')dz'} = 1$$

$$t = e^{-i\left(\int\limits_{0}^{z_0} p(z')dz' + \int\limits_{z_0}^{z_1} p(z')dz' + \int\limits_{z_1}^{0} p(z')dz'\right)}$$

Для нахождения r выберем разрез вдоль линии анти-Стокса. Снизу обходим разрез около точки $z_1 = e^{i\frac{\pi}{4}}$ ($\arg_{z=z_1} z_1 = \frac{13}{12}\pi$) и получим

$$C_- e^{-\frac{i}{4}\frac{13}{12}\pi} e^{-i|\xi|^{3/2}|z_0|^{3/2}\frac{\sqrt{2mU_0}}{3a^2}} + C_+ e^{-\frac{i}{4}\frac{13}{12}\pi} e^{i|\xi|^{3/2}|z_0|^{3/2}\frac{\sqrt{2mU_0}}{3a^2}} =$$

$$= C_- e^{\frac{i}{4}\frac{11}{12}\pi} e^{i|\xi|^{3/2}|z_0|^{3/2}\frac{\sqrt{2mU_0}}{3a^2}} + C_+ e^{\frac{i}{4}\frac{11}{12}\pi} e^{-i|\xi|^{3/2}|z_0|^{3/2}\frac{\sqrt{2mU_0}}{3a^2}}$$

Нижний берег разреза:

$$\psi = t\psi_+ \to C_- = it, \quad C_+ = 0$$

По верхнему берегу разреза вдоль линии анти-Стокса переходим к $z_1 = e^{i\frac{3\pi}{4}}$, и обходим сверху. C_+ остается 0, при пересечении первой линии Стокса из постоянства C_+ следует также сохранение C_-. Вторая линия анти-Стокса с ψ_--доминированием. Пользуемся условие сшивки на действительной оси и получаем

$$r = ite^{-i\sqrt{2mU_0}\left(\int\limits_{z_1}^{0} + \int\limits_{z_0+0}^{z_1+0} + \int\limits_{0}^{z_0}\right)\sqrt{\alpha+\frac{z^4}{a^4}}dz}$$

- Коэффициент прохождения:

$$t = 1$$

$$\sqrt{\alpha + \frac{z^4}{a^4}} = e^{\frac{i}{2}\cdot 2\pi}\sqrt{\alpha + \frac{z^4}{a^4}}$$

$$\left(\int\limits_{z_1-0}^{z_0-0} + \int\limits_{z_0+0}^{z_1+0}\right)\sqrt{\alpha + \frac{z^4}{a^4}}dz = 2\int\limits_{z_1-0}^{z_0-0}\sqrt{\alpha + \frac{z^4}{a^4}}dz$$

Из голоморфности функций:

$$\int\limits_{z_1-0}^{z_0-0}\sqrt{\alpha + \frac{z^4}{a^4}}dz = \int\limits_{z_1}^{0}\sqrt{\alpha + \frac{z^4}{a^4}}dz + \int\limits_{0}^{z_0}\sqrt{\alpha + \frac{z^4}{a^4}}dz$$

$$\left(\int\limits_{z_1-0}^{z_0-0} + \int\limits_{z_0+0}^{z_1+0}\right)\sqrt{\alpha + \frac{z^4}{a^4}}dz = -2i\cos\frac{\pi}{4}a\alpha^{3/4}\int\limits_{0}^{1}\sqrt{1-t^4}dt = -2i\cos\frac{\pi}{4}a\alpha^{3/4}\frac{\Gamma(1/4)^2}{6\sqrt{2\pi}}$$

$$r = i\exp\Big[-2a\sqrt{mE\sqrt{\frac{E}{U_0}}}\frac{\Gamma(1/4)^2}{6\sqrt{2\pi}}\Big]$$

17.3.4 Problems about basic 1D scatterings 1

O3.1-3.12 Scattering over a pot

Найти волновую функцию и уровни энергии стационарных состояний частицы массой m, локализованной в симметричной одномерной потенциальной яме прямоугольной формы, глубина которой равна U_0, а ширина $2a$.

Solution

Примем за начало координат центр дна ямы O (см. рис. 19 к условию задачи). Тогда уравнение Шредингера для связанных состояний внутри ямы будет

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \tag{1}$$

а вне ямы

$$\frac{d^2\psi}{dx^2} - \alpha^2\psi = 0 \tag{2}$$

где введены обозначения

$$k = \sqrt{\frac{2m\ell}{\hbar^2}}, \quad \alpha = \sqrt{\frac{2m\,(U_0 - \mathscr{E})}{\hbar^2}} \tag{3}$$

Внутри ямы общее решение имеет вид

$$\psi = A\cos kx + B\sin kx.$$

Вне ямы решение, удовлетворяющее условиям на бесконечности $\Psi(\pm\infty) \to 0$, будет

$$\begin{aligned} \psi &= Ce^{-\alpha x} \quad \text{при} \quad x > a, \\ \psi &= De^{\alpha x} \quad \text{при} \quad x < -a. \end{aligned}$$

Из соображений симметрии следует, что плотность вероятности $|\psi|^2$ должна быть симметричной функцией x относительно начала координат. Следовательно, должно быть $C^2 = D^2$, т. е. возможны два случая: $C = D$ и $C = -D$. Постоянные A, B, C, D надо выбрать так, чтобы на краях ямы функция ψ и ее производная $d\psi/dx$ были непрерывны. На границе $x = +a$ это дает

$$\begin{aligned} A\cos ka + B\sin ka &= Ce^{-\alpha a} \\ -kA\sin ka + kB\cos ka &= -\alpha Ce^{-\alpha a} \end{aligned}$$

а на границе $x = -a$

$$\begin{aligned} A\cos ka - B\sin ka &= De^{-\alpha a} \\ kA\sin ka + kB\cos ka &= \alpha De^{-\alpha a} \end{aligned}$$

Отсюда

$$\begin{aligned} 2A\cos ka &= (C + D)e^{-\alpha a}, \quad 2kA\sin ka = \alpha(C + D)e^{-\alpha a} \\ 2B\sin ka &= (C - D)e^{-\alpha a}, \quad 2kB\cos ka = -\alpha(C - D)e^{-\alpha a} \end{aligned}$$

Если $A \neq 0$ и $C = D$, то

$$k\,\mathrm{tg}\,ka = \alpha \tag{4}$$

Если же $B \neq 0$ и $C = -D$, то

$$k\,\mathrm{ctg}\,ka = -\alpha \tag{5}$$

Эти условия не могут быть удовлетворены одновременно, так как в противном случае получилось бы $k^2 = -\alpha^2$, а это невозможно ввиду вещественности k и α. Решение, когда все коэффициенты A, B, C, D равны нулю, физического смысла не имеет. Таким образом, все возможные решения разделяются на два класса: решения с четной волновой функцией, когда $A \neq 0, B = 0, C = D$ и решения с нечетной волновой функцией, когда $A = 0, B \neq 0, C = -D$.

Уровни энергии найдутся путем графического или численного решения уравнения (4) или уравнения (5), в которых положительные величины k и α определяются выражениями (3). Для графического решения удобно ввести безразмерные величины

$$\xi = ak, \quad \eta = a\alpha \tag{6}$$

Тогда

$$\xi^2 + \eta^2 = \frac{2mU_0a^2}{\hbar^2} \tag{7}$$

причем для решений с четной волновой функцией

$$\eta = \xi\,\mathrm{tg}\,\xi \tag{4a}$$

а для решений с нечетной волновой функцией

$$\eta = -\xi \operatorname{ctg} \xi \tag{5a}$$

На рис. 145a построены кривые $\eta = \xi \operatorname{tg} \xi$, на рис. 145б - кривые $\eta = -\xi \operatorname{ctg} \xi$.

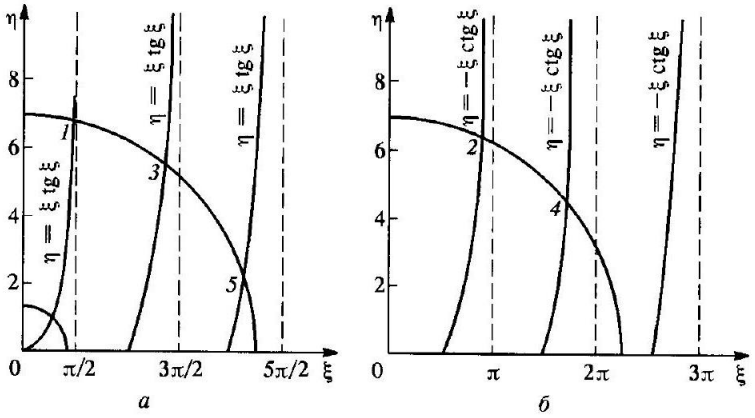


Рис. 145

Вертикальными штриховыми линиями изображены асимптоты этих кривых. Ввиду положительности ξ и η нужны только участки этих кривых, расположенные в положительном квадранте ($\xi > 0, \eta > 0$). Пересечем эти кривые окружностью (7), радиус которой $\sqrt{2mU_0}a/\hbar$ должен

считаться известным. Координаты точек пересечения этой окружности с кривыми (4а) и (5а) дадут возможные значения ξ и η. После этого по формулам (3) легко найти значения $\mathscr{E}$. Число уровней всегда конечно и определяется глубиной U_0 и шириной $2a$ потенциальной ямы. Например, если радиус окружности равен 7, то получается пять уровней. Точкам пересечения $1, 3, 5$ соответствуют четные, а точкам 2 , 4 - нечетные волновые функции. Если $0 \leqslant U_0 a^2 \leqslant \hbar^2\pi^2/8m$, то имеется только одна точка пересечения, которой соответствует четная волновая функция.

Следует еще раз подчеркнуть, что в симметричной одномерной яме при любой ее глубине и ширине всегда есть хотя бь один уровень, отвечающий четной ψ-функции. Аналогично обстоит дело в двумерном случае. Принципиально по-другому обстоит дело в случае трехмерной потенциальной прямоугольной ямы (задача 3.16*), где уровень есть не всегда.

Дадим также другой способ решения уравнений (4) и (5).

Рассмотрим четное решение $k \operatorname{tg} ka = \alpha$, откуда $1 + \operatorname{tg}^2 ka = \frac{\alpha^2+k^2}{k^2}$;

$$\frac{1}{\cos^2 ka} = \frac{2mU_0a^2}{\hbar^2}\frac{1}{(ka)^2}; |\cos ka| = \sqrt{\frac{\hbar^2}{2mU_0a^2}}ka$$

При этом (т.к. $\operatorname{tg} ka > 0$) годятся те четверти, где $\sin ka$ и $\cos ka$ имеют одинаковые знаки.

Для нечетного решения получаем $|\sin ka| = \sqrt{\frac{\hbar^2}{2mU_0a^2}}ka$, и т.к. $\operatorname{ctg} ka < 0$, то годятся те четверти, где $\sin ka$ и $\cos ka$ имеют разные знаки. Графическое решение полученных уравнений изображено на рис. 146 и 147.

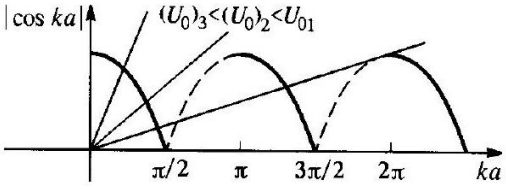


Рис. 146

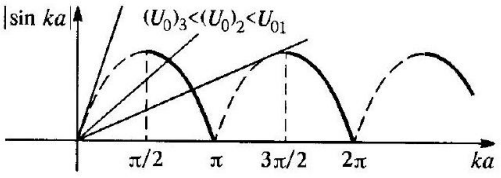


Рис. 147

Видно, что в зависимости от величины U_0 (при данном a) или a (при данном U_0) в случае четной ψ-функции хотя бы одно решение есть всегда! Это будет иметь место при $\sqrt{\frac{\hbar^2}{2mU_0a^2}} > \frac{1}{\pi/2} = \frac{2}{\pi}$, или $U_0 a > \frac{\pi^2\hbar^2}{8m}$. При дальнейшем уменьшении U_0 уровень поднимается к потолку ямы, но частица из ямы не вылетает (рис. 148)!

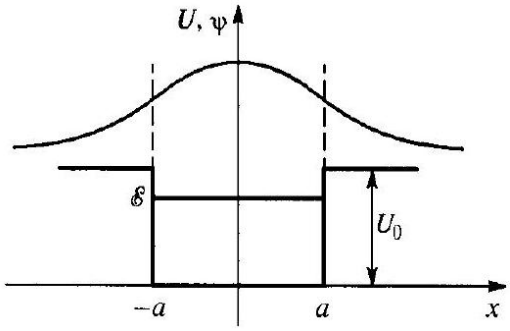


Рис. 148

О3.1-3.1

Найти плотность потока вероятности для:
а) плоской волны $\psi = \exp\left(i\frac{p_z}{\hbar}z\right) = \exp(ikz)$,
б)сферической волны $\psi = \frac{1}{kr}\exp(ikr)$,
в) суммы сходящейся и расходящейся волн $\psi = \frac{1}{2kr}\left(se^{ikr} - e^{-ikr}\right)$.

3.

1. Решение. Плотность потока вероятности вычисляется по формуле

$$\mathbf{j} = \frac{i\hbar}{2m}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right)$$

или в одномерном случае

$$j_z = \frac{i\hbar}{2m}\left(\psi\frac{\partial\psi^*}{\partial z} - \psi^*\frac{\partial\psi}{\partial z}\right) \qquad (*)$$

а) В случае плоской волны $\psi(z) = \mathrm{e}^{ikz}$ плотность потока вероятности определим прямой подстановкой волновой функции в (*):

$$j_z = \frac{\hbar k}{m} = v$$

т. е. равна скорости частицы v.
б) В случае сферической расходящейся волны $\psi(r) = \frac{1}{kr}\mathrm{e}^{ikr}$, очевидно, вектор плотности потока вероятности $\mathbf{j}$ направлен по радиусу-вектору $\mathbf{r}$. Кроме того будем считать $kr \gg 1$. Поэтому

$$\mathbf{j} = \frac{\hbar k}{m}\frac{1}{(kr)^2}\frac{\mathbf{r}}{r} = \frac{v}{(kr)^2}\frac{\mathbf{r}}{r} = \frac{\mathbf{v}}{(kr)^2}$$

В последнем равенстве учтено, что k || r || v. Можно было бы воспользоваться декартовыми координатами, направив ось z по радиусу-вектору. Естественно, ответ получился бы таким же:

$$j_z = \frac{v_z}{(kr)^2}$$

в) Для суммы сходящейся и расходящейся волновых функций приведем только ответ:

$$\mathbf{j} = \frac{\mathbf{v}}{(2kr)^2}\left(|s|^2 - 1\right)$$

О3.1-3.2

Волновая функция частицы массой m, совершающей одномерное движение, имеет вид $\psi(x) = Ae^{-\alpha x^2}$. Найти потенциал $U(x)$, в котором двигается частица, и ее энергию $\mathcal{E}$ что при $x = 0, U(x) = 0$.

Solution.

$U(x) = \frac{2\alpha^2\hbar^2}{m}x^2$ (гармонический осциллятор), $\mathscr{E} = \frac{\alpha\hbar^2}{m}$.
Указание: в задачах 3,2; 3, 3; 3, 4 предпочтительнее не интегрировать по частям, а наоборот - дифференцировать по параметру α определенный интеграл $\int_0^\infty \mathrm{e}^{-\alpha x}dx = \frac{1}{\alpha}$.

О3.1-3.3

Волновая функция частицы массой m, совершающей одномерное движение в поле с потенциалом $U(x)$, есть

$$\psi(x) = \begin{cases} \Lambda x^2 \exp(-x/a) & \text{при } x > 0 \\ 0 & \text{при } x \leqslant 0 \end{cases}$$

Оценить с помощью соотношения неопределённостей среднюю кинетическую энергию $\langle T \rangle$ частицы и сравнить с результатом точного расчета. Найти $U(x)$ при $x > 0$ и полную энергию частицы $\mathscr{E}$, если известно, что $U(x) \to 0$ при $x \to \infty$.

3.

3. $\langle T \rangle \approx \frac{\hbar^2}{32ma^2}$ (точное значение $\langle T \rangle = \frac{\hbar^2}{6ma^2}\Big)$; $U(x) = \frac{\hbar^2}{m}\left(\frac{1}{x^2} - \frac{2}{ax}\right)$; $\mathscr{E} = -\frac{\hbar^2}{2ma^2}$ (см. указание к задаче 3.2).

О3.1-3.4 Все по волновой функции

Волновая функция частицы массой m, совершающей одномерное движение в поле с потенциалом $U(x)$, есть

$$\psi(x) = \begin{cases} Ax \exp(-x/a) & \text{при } x > 0 \\ 0 & \text{при } x \leqslant 0. \end{cases}$$

Оценить с помощью соотношения неопределённостей среднюю кинетическую энергию $\langle T \rangle$ частицы и сравнить с результатом точного расчета. Найти среднее значение координаты $\langle x \rangle$, а также $U(x)$ при $x > 0$ и полную энергию $\circ$, если известно, что $U(x) \to 0$ при $x \to \infty$.

Solution.

Заметьте, что дана именно волновая функция, а не потенциал!
Плотность вероятности найти частицу:

$$w(x) = \psi^* \psi = A^2 x^2 \exp\left(-\frac{2x}{a}\right) \text{ при } x \geq 0$$

Найдем максимум:

$$\frac{dw(x)}{dx} = 0 \to x_m = a$$

Тогда неопределенность по координате как $2a$ - влево и вправо от максимума. Тогда из соотношения неопределённостей:

$$p \approx \Delta p = \frac{\hbar}{2a} \to \langle T \rangle = \frac{p^2}{2m} = \frac{\hbar^2}{8ma^2}$$

3.4. $\langle T \rangle \approx \frac{\hbar^2}{8ma^2}$ (точное значение $\langle T \rangle = \frac{\hbar^2}{2ma^2}\Big)$; $\langle x \rangle = \frac{3}{2}a; U(x) = -\frac{\hbar^2}{max}$; $\mathscr{E} = -\frac{\hbar^2}{2ma^2}$ (см. указание к задаче 3.2).

О3.1-3.5

Частица массы m находится в одномерном потенциале

$$U(x) = \begin{cases} \infty & \text{при } x < 0, \\ kx & \text{при } x > 0. \end{cases}$$

Оценить энергию основного состояния частицы в этом потенциале, используя в качестве волновой функции $\psi = x\exp(-ax)$. В качестве оценки взять минимальное значение среднего значения полной энергии частицы. Сравнить с задачей 2.39.

3.

5. $\mathscr{E}_0 \approx \left(\frac{9}{4}\frac{\hbar^2 k^2}{m}\right)^{1/3}$, параметр $a = \left(\frac{3mk}{2\hbar^2}\right)^{1/3}$. См. также задачу 2.39. Полученный ответ совпадает с точным решением с точностью 6%.

О3.1-3.6

Используя правило квантования Бора-Зоммерфельда, найти закон квантования энергии частицы массой m при больших значениях главного квантового числа n (в квазиклассическом приближении) в одномерном потенциале

$$U(x) = \begin{cases} \infty & \text{при} \quad x < 0 \\ kx & \text{при} \quad x > 0 \end{cases}$$

У к а з а н и е. Правило квантования Бора-Зоммерфельда: $\oint \mathbf{p} d\mathbf{l} = nh$.

3.

6. $\mathscr{E}_n = \frac{3}{2}\sqrt[3]{\frac{k^2\pi^2\hbar^2}{m}} n^{2/3}$.

(?? заново нужно решать!)

$$dx = \frac{-pdp}{km}$$

$$2\int_{p_0}^{0} \frac{p^2}{km} dp = \frac{2}{3}\frac{p_0^3}{km} = 2\pi\hbar h$$

дальше находим p_0

$$p_0 = [2\pi\hbar k m \frac{2}{3}]^{1/3} n^{1/3}$$

он зависит как корень 3 степени из n????
дальше $E_n \sim n^{2/3}$, $\frac{\Delta E}{E} \sim \frac{\Delta n}{n}\frac{2}{3}$
??????

О3.1-3. 7

В кулоновском поле простейшим сферически симметричным решением уравнения Шрезингера является волновая функция $\psi = A\exp(-ar)$. Какой энергии (в эВ) соответствует это состояние для электрона в кулоновском поле ядра с зарядом $Z = 10$? Чему равна a?

3.

7. $\mathscr{E} = -\frac{mZ^2\mathrm{e}^4}{2\hbar^2} = -1,36\kappa$ В; $a = \frac{\hbar^2}{Zm\mathrm{e}^2} = 0,053$Å.

О3.1-3. 8

Взаимодействие между нуклонами в дейтроне может быть описано потенциалом Юкавы $U(r) = -U_0\frac{\exp(-r/a)}{r/a}$, где r - относительное расстояние, a - радиус взаимодействия ядерных сил, $U_0 = 40$МВ. Если аппроксимировать волновую функцию основного состояния как водородоподобную $\psi(r,\alpha) = \sqrt{\frac{\alpha^3}{8\pi a^3}}\exp\left(-\frac{\alpha r}{2a}\right)$, где a - параметр, при котором достигается минимальная энергия основного состояния, то энергия связи оказывается равной $\mathcal{E}_0 = -1,08$МВ. Определить величину a.

Ук а з а н и е. Уравнение $\frac{x^3(x-1)}{(1+x)^3} = 0,108$ имеет корень $x = 1,5$.

3.

8. $a = \hbar\sqrt{\frac{(1+\alpha)^3}{2\mu U_0\alpha(\alpha+3)}} \approx 1,54\cdot 10^{-13}$ cm.

Решение. Учитывая сферическую симметрию задачи, запишем

$$\langle\mathscr{E}\rangle = \langle T+U\rangle = \int_0^\infty \psi^*\left[\frac{\hat{p}^2}{2\mu} + U(r)\right]\psi dV,$$

где $dV = 4\pi r^2 dr; \mu = m_N/2$ - приведенная масса дейтрона. Оператор

$$\hat{p}^2 = -\hbar^2\Delta_r = -\hbar^2\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)$$

Вычисляя интегралы, получаем

$$\langle\mathcal{G}\rangle = \frac{\hbar^2\alpha^2}{8\mu a^2} - U_0\frac{a^3}{(1+\alpha)^2}.$$

Основное состояние соответствует минимуму энергии:

$$\frac{d\langle\mathfrak{G}\rangle}{d\alpha} = 0, \text{ откуда } \frac{(1+\alpha)^3}{\alpha(3+\alpha)} = \frac{2\mu a^2 U_0}{\hbar^2}.$$

Далее находим

$$\mathscr{E}_0 = \langle\mathscr{E}\rangle = \frac{\alpha^3(1-\alpha)}{(1+\alpha)^3}\frac{U_0}{4} \text{ или } \frac{\alpha^3(1-\alpha)}{(1+\alpha)^3} = 0,108.$$

Используя указание к задаче, находим, что $\alpha = 1,5$. Таким образом,

$$a = \hbar\sqrt{\frac{(1+\alpha)^3}{2\mu U_0\alpha(\alpha+3)}} \approx 1,54\cdot 10^{-13} \text{ cm}.$$

О3.1-3.9. Энергия связи дейтрона, зная потенциал (???)

Взаимодействие между нуклонами в дейтроне может быть описано потенциалом $U(r) = -U_0\exp\left(-\frac{r}{a}\right)$, где $U_0 = 32,7$ МэВ, $a = 2,2$ фм, r - расстояние между нуклонами. Аппроксимируя волновую функцию основного состояния водородоподобной $\psi(r,\alpha) = \sqrt{\frac{\alpha^3}{8\pi a^3}}\exp\left(-\frac{\alpha r}{2a}\right)$, где α - параметр, при котором достигается минимум энергии основного состояния, найти энергию связи дейтрона.

У к а з а н и е. Уравнение $\frac{(1+x)^4}{x} = 22,6$ имеет корень $x = 1,35$.

3.

9. $\langle E(\alpha)\rangle = \frac{\hbar^2\alpha^2}{8\mu a^2} - U_0\frac{\alpha^3}{(1+\alpha)^3} \approx -2,2$ МэВ, где $\alpha = 1,35$.

О3.1-3.10 Волновая функция трехмерного осциллятора (?)

Волновая функция трехмерного изотропного осциллятора, характеризуемого классической частотой ω и приведенной массой μ, имеет вид $\psi = A\left(1+\alpha r^2\right)e^{-\beta r^2}$, где A, α и β - некоторые константы. Определить величину констант α и β, энергию этого состояния и главное квантовое число. Смотрите также задачу 4.10.

3.

10: 1) $\alpha = -\frac{2}{3}\frac{\mu\omega}{\hbar}; \beta = \frac{\mu\omega}{2\hbar}; \mathscr{E} = \frac{7}{2}\hbar\omega$, поскольку $\mathscr{E}_N = \hbar\omega\left(N+\frac{3}{2}\right)$, то $N = 2$.
2) $\alpha = 0; E = \frac{3}{2}\hbar\omega, N = 0$.

Решение. В трехмерном случае в сферических координатах (r,θ,φ) лапласиан Δ имеет вид

$$\Delta = \Delta_r + \frac{1}{r^2}\Delta_{\theta,\varphi}.$$

Поскольку ψ-функция не зависит от углов (сферически симметричный случай, изотропный осциллятор), то лапласиан в нашей задаче сводится к радиальной части Δ_r

$$\Delta = \Delta_r \equiv \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}.$$

Дифференцируя исходную ψ-функцию, получим

$$\frac{d\psi}{dr} = 2Ae^{-\beta r^2}\left[(\alpha-\beta)r - \alpha\beta r^3\right]$$
$$\frac{d^2\psi}{dr^2} = 2Ae^{-\beta r^2}\left[2\alpha\beta^2 r^4 - \beta(5\alpha-2\beta)r^2 + (\alpha-\beta)\right]$$

Таким образом, уравнение Шредингера имеет вид

$$-\frac{\hbar^2}{2\mu}\left(\frac{d^2\psi}{dr^2}+\frac{2}{r}\frac{d\psi}{dr}\right)+\frac{\mu\omega^2}{2}r^2\psi=\mathscr{E}\psi,\ \text{или}$$

$$-6\beta+4\beta^2r^2-14\alpha\beta r^2+4\alpha\beta^2r^4+6\alpha-$$
$$-\frac{\mu^2\omega^2}{\hbar^2}r^2-\frac{\mu^2\omega^2}{\hbar^2}r^4\alpha=-\frac{2\mu}{\hbar^2}\S-\frac{2\mu}{\hbar^2}£\alpha r^2.$$

Поскольку энергия $\mathscr{E}=\text{const}$ и не может зависеть от r, то сумма коэффициентов при всех степенях r должна давать 0 .

$$\begin{array}{ll} r^0: & 6(\alpha-\beta)+\frac{2\mu}{\hbar^2}\mathscr{E}=0 \\ r^2: & -14\alpha\beta+4\beta^2-\frac{\mu^2\omega^2}{\hbar^2}+\frac{2\mu\mathscr{E}}{\hbar^2}\alpha=0, \\ r^4: & 4\alpha\beta^2-\frac{\mu^2\omega^2}{\hbar^2}\alpha=0. \end{array}$$

Из этой системы и следуют искомые значения α,β, $\mathscr{E}$ и N, приведенные в ответе.

О3.1-3.11

Найти волновую функцию и уровни энергии стационарных состояний частицы массой m, локализованной в одномерной потенциальной яме прямоугольной формы с бесконечно высокими стенками. Ширина ямы равна $2a$.

3.

11. $\Psi=\begin{cases}\frac{1}{\sqrt{a}}\cos\frac{n\pi x}{2a} & (n=1,3,5,\ldots),\\ \frac{1}{\sqrt{a}}\sin\frac{n\pi x}{2a} & (n=2,4,6,\ldots),\end{cases}\quad \mathscr{E}=\frac{\hbar^2\pi^2}{8ma^2}n^2$ в обоих случаях.

Вследствие симметричности потенциала решения подразделяются на четные и нечетные. В силу граничных условий ($\Psi(\pm a)=0$) на ширине ямы должно укладываться целое число полуволн де Бройля, как это имеет место для электромагнитных волн в случае интерферометра Фабри-Перо или волновода с металлическими стенками.

(типичная элементарная задача, должен решать за 1 минуту, потом потренируюсь, нужно 1ю часть прописать без херни.)

О3.1-3.13 Сила давления и энергия электронов в яме (!!!)

В одномерной потенциальной яме шириной b с бесконечными стенками находятся N электронов. Определить минимальное значение полной энергии $\mathscr{E}_{\min}$ и силу F давления электронов на стенки ямы. Взаимодействием электронов пренебречь.

3.

13. $\mathscr{E}_{\min}=\frac{\pi^2\hbar^2}{4mb^2}\frac{N(N+2)(N+1)}{6}; F=\frac{\pi^2\hbar^2}{2mb^3}\frac{N(N+2)(N+1)}{6}$.

О3.1-3.14

Поток свободно распространяющихся нейтронов падает на непроницаемую стенку толщиной L, в которой имеется канал прямоугольного поперечного сечения с высотой $d=10^{-3}$см и шириной $l\gg d$. Длина канала $L\gg l$ (рис. 20). При каких значениях скорости v нейтронов в падающем пучке нейтроны могут пройти сквозь канал? Чему равна минимальная скорость $v_{\min}$ в случае квадратного сечения канала $d\times d$?

3.

14. Вообще $v>\frac{\pi\hbar}{mdl}\sqrt{d^2+l^2}$. При $d\ll l v_{\min}=\frac{\pi\hbar}{md}\approx 2$ cm/c.
При $d=l$ (квадратное сечение канала) $v_{\min}=\frac{\sqrt{2}\pi\hbar}{md}\approx 2,8$ cm/c.

(такая же, как и следующая задача, только уровни энергии еще по перпендикулярному состоянию)

О3.1-3.15 Пролет нейтронов через щель (???)

Поток нейтронов, летящих со скоростью $V_0 = 25$см/ сек, падает на широкую щель с абсолютно отражающими стенками. Длина щели $l = 1$см, высота $d = 10^{-4}$см. Сколько времени нейтрон будет находиться внутри щели, если он в нее попадет?

3.

15. $t = 0,065$ с.

(?? идейно не очень понимаю, как все тут работает???)
(!!! в 1ю часть добавлю очевидные формулы для этой задачи)
Качественно такое описание. Энергия тратится на отражения, поэтому скорость в этой щели меньше. нулевой уровень:

$$E_0 = \frac{\pi^2\hbar^2}{2md^2}$$

Закон сохранения энергии:

$$\frac{mv_0^2}{2} = \frac{mv^2}{2} + \frac{\pi^2\hbar^2}{2md^2}$$

можно найти

$$v = \sqrt{v_0 - \frac{\pi^2\hbar^2}{2md^2}}$$

ответ: $t = \frac{l}{v} = 0.066$ с.

О строгом описании (???)

(?? почему вообще закон сохранения энергии так выполняется??? что-то сомнительное вроде решение. мб 1ю часть доработаю потом тоже.)

О3.1-3.16

В трехмерной прямоугольной потенциальной яме

$$U(r) = \begin{cases} -U_0 & \text{при} \quad r < a, \\ 0 & \text{при} \quad r > a. \end{cases}$$

Найти волновые функции и энергии стационарных состояний при нулевом моменте импульса.

3.

16. Решение. В сферической системе координат уравнение Шредингера для стационарных состояний с волновыми функциями, зависящими только от r, имеет вид

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) + \frac{2m}{\hbar^2}[\mathscr{E} - U(r)]\psi = 0 \tag{1}$$

Решение этого уравнения должно быть конечным при $r = 0$ и достаточно быстро убывать при $r \to \infty$ (чтобы $\int |\psi|^2 dV$ сходился). Введем новую функцию $\chi = r\psi$. Тогда

$$\frac{d^2\chi}{d^2r} + \frac{2m}{\hbar^2}[\mathscr{E} - U(r)]\chi = 0 \tag{2}$$

Надо найти решения этого уравнения, убывающие при $r \to +\infty$ и обращающиеся в нуль при $r = 0$. Это будут

$$\begin{array}{ll} \chi = B\sin kr & \text{при } r \leqslant a, \\ \chi = Ce^{-\alpha r} & \text{при } r \geqslant a, \end{array}$$

где

$$k = +\sqrt{\frac{2m\,(\mathscr{E} + U_0)}{\hbar^2}}, \quad \alpha = +\sqrt{-\frac{2m\mathscr{E}}{\hbar^2}}. \tag{3}$$

Задача свелась к задаче об одномерной потенциальной яме - уровни энергии определяются точно так же, надо только отбросить состояния с четными и сохранить состояния лишь с нечетными волновыми функциями.

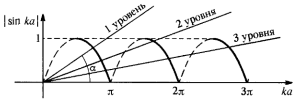
О3.1-3.17 Уровень в 3D кубе (!!!????)

Частица массой m локализована в трехмерной потенциальной яме прямоугольной формы, радиус которой равен . Определить минимальную глубину ямы U_0, при которой появится первый уровень энергии. Чему равна энергия частицы $\mathcal{E}$ на этом уровне?

Solution.

3.17. Решение задачи сводится к решению трансцендентного уравнения $|\sin ka| = \sqrt{\frac{\hbar^2}{2mU_0a^2}}ka$, где $k^2 = \frac{2m(U_0-\varkappa)}{\hbar^2}$, (см. рис. 149).

Минимальная «мощность» U_0a^2 ямы, при которой появляется первый уровень, $U_0a^2 = \pi^2\hbar^2/(8m)$. При этом энергия уровня ($ka = \pi/2$) равна $\mathscr{E} = 0$, т. е. уровень лежит на «потолке» ямы. При увеличении U_0 или a уровень опускается в яму. Из рис. 149 видно, что второй уровень появится при $\operatorname{tg}\alpha = \frac{2}{3\pi}$; третий - при $\operatorname{tg}\alpha = \frac{2}{5\pi}$ и т. д. Итак, $U_0 = \frac{\pi^2\hbar^2}{8ma^2}$.



17.3.5 Problems about basic 1D scatterings 2

О3.1-3.18 Моделирование дейтрона

Дейтрон - это ядро дейтерия, состоящее из протона и нейтрона. Энергия связи дейтрона, измеренная экспериментально, равна $\mathscr{E} = 2,225$ МэВ. Аппроксимируя потенциальную энергию взаимодействия протона с нейтроном с помощью трехмерной прямоугольной потенциальной ямы, определить ее глубину U_0, при которой возможно такое связанное состояние. Радиус потенциальной ямы $a = 1,6 \cdot 10^{-13}$см.

3.

18. $U_0 = \frac{\pi^2\hbar^2}{8\mu a^2} + \mathscr{E} \approx$ 42М ЭВ, где $\mu = \frac{m_p}{2}$. Это довольно грубая оценка. Точное решение трансцендентного уравнения дает $U_0 \approx$ 53М ВВ. Смотрите задачу 3.17 .

О3.1-3.19

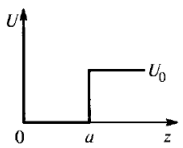
Определить среднее значение квадрата импульса $\langle p^2\rangle$ и среднее значение квадрата координаты $\langle x^2\rangle$ частицы массой m, находящейся в одномерной «мелкой» $\left(U_0 \ll \hbar^2/ma^2\right)$ симметричной потенциальной яме, изображенной на рис. 23. Проверить выполнение соотношения Гайзенберга $\langle p^2\rangle\langle x^2\rangle \geqslant \hbar^2/4$.

3.

19. $\left\langle x^2\right\rangle = \frac{\hbar^4}{8m^2a^2U_0^2}; \left\langle p^2\right\rangle = \frac{4m^2a^2U_0^2}{\hbar^2}; \left\langle x^2\right\rangle\left\langle p^2\right\rangle = \frac{\hbar^2}{2} \Big\rangle \frac{\hbar^4}{2}$.

О3.1-3.20 Средняя координата в яме у стенки

Потенциальную энергию взаимодействия $U(z)$ атома гелия с плоской поверхностью твердого тела $z = 0$ можно аппроксимировать прямоугольной ямой некоторой глубины U_0 и шириной $a = 5$Å, причем $U(z = 0) = +\infty$ (рис. 24). Полагая, что волновая функция адсорбированного атома в основном состоянии достигает максимума при $z = 0,99a$, найти среднее значение координаты $\langle z\rangle$ для адсорбированных атомов в основном состоянии.



Solution.

(??? я уже решал ее из Гольдмана Кривченкова, еще раз допишу суть!)

3.20*. $\langle z\rangle \approx \dfrac{2a}{\pi^2\delta} \approx 20a = 100\text{Å}$, где $\delta = 0,01$ (точное значение $\langle z\rangle =$
$=\dfrac{4a}{\sqrt{2}\pi^2\delta} \approx 140\text{Å}$).

Решение. Разобьем область нахождения атома гелия на две части: I внутри потенциальной ямы $(0 < z \leqslant a)$ и II - вне ее при $z > a$. В области I:
Решение этого дифференциального уравнения очевидно:

$$\psi_1(z) = \sin kz, \quad \text{поскольку при } z = 0 \text{ должно быть } \psi_1(0) = 0.$$

В области I:

$$\psi''_{\text{II}} - \varkappa^2\psi_{\text{II}} = 0, \text{ где } \quad x = \frac{1}{\hbar}\sqrt{2m\,(U_0 - \mathscr{E})}$$

Решение последнего уравнения

$$\psi_{\text{II}}(z) = Ae^{-xz}$$

где A - нормировочная константа. Заметим, что формальным решением этого уравнения могла бы быть положительная экспонента $\propto \exp(xz)$. Но тогда при $z \to \infty, \psi(z) \to \infty$, что не имело бы физического смысла.
На границе областей, т. е. при $z = a$ необходима гладкая сшивка ψ-функций:

$$\psi_{\text{I}}(a) = \psi_{\text{II}}(a), \text{ т. е. } \sin ka = Ae^{-\varkappa a}$$
$$\psi'_{\text{I}}(a) = \psi'_{\text{II}}(a), \text{ т. е. } k\cos ka = -A\varkappa e^{-\varkappa a}$$

Откуда следует

$$\operatorname{ctg} ka = -\frac{x}{k}$$

По условию волновая функция адсорбированного атома в основном состоянии достигает максимума при $z = z^* = 0,99a = (1-\delta)a$, где $\delta = 0,01$. Максимум лежит в области I, т. е.

$$\psi_1(z^*) = \sin kz^* = 1, \text{ откуда } kz^* = \frac{\pi}{2}$$

и откуда определим k:

$$k = \frac{\pi}{2z^*} = \frac{\pi}{2(1-\delta)a} \approx \frac{\pi}{2a}(1+\delta)$$

Вычислим

$$\operatorname{ctg} ka = \frac{\cos\left(\frac{\pi}{2} + \frac{\pi\delta}{2}\right)}{\sin\left(\frac{\pi}{2} + \frac{\pi\delta}{2}\right)} = -\sin\frac{\pi\delta}{2} \approx -\frac{\pi\delta}{2}$$

Из соотношения (3) определим x:

$$x = -k\operatorname{ctg} ka \approx k\frac{\pi\delta}{2} = \frac{\pi^2}{4a}\delta \simeq 5\cdot 10^5 \text{ cm}^{-1}$$

По определению

$$\langle z\rangle = \frac{\int\limits_0^a z\sin^2 kzdz + \int\limits_a^\infty A^2e^{-2xz}zdz}{\int\limits_0^a \sin^2 kzdz + \int\limits_a^\infty A^2e^{-2xz}dz}$$

Но интегралами по области I можно пренебречь в силу их малого вклада, одновременно расширив область интегрирования в области II до 0. Действно, $\frac{\int\limits_0^\infty ze^{-2xz}dz}{\int\limits_0^\infty -2xz} = \frac{1}{2x}$, но $\frac{\int\limits_a^\infty ze^{-2xz}dz}{\int\limits_\infty^\infty -2xz} = \frac{1+2xa}{2x}$. Так как $2xa \approx 10^{-2}$, то

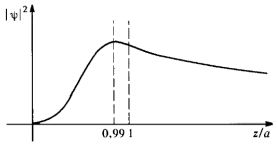
$$\int\limits_0 e^{-2xz}dz \quad \int\limits_a e^{-2xz}dz$$

это очень близкие выражения. Поэтому

$$\langle z\rangle \approx \frac{\int\limits_0^\infty ze^{-2xz}dz}{\int\limits_0^\infty e^{-2xz}dz} = \frac{1}{2x} = \frac{2a}{\pi^2\delta} \approx 20a = 100\text{Å}$$

На рис. 150 приведен график зависимости $|\psi(z)|^2$. Хотя максимум ψ функции и лежит внутри потенциальной ямы, но среднее значение координаты $\langle z\rangle$ - далеко за ее пределами, поскольку ψ-функция крайне медленно спадает при $z > a$. Точное интегрирование дает

$$\langle z\rangle = \frac{2\sqrt{2}a}{\pi^2\delta} \approx 140\text{Å}$$



O3.1-3.21

Энергия взаимодействия $U(z)$ атома водорода с твердой стенкой аппроксимируется прямоугольной потенциальной ямой глубиной U_0, шириной $a = 6$Åи $U(z = 0) = +\infty$ (рис. 25). Энергия адсорбции - это разность наинизших уровней свободного и прилипшего к стенке атома $\mathscr{E} = U_0 - \mathscr{E}_1 = 1$ K. Найти величину U_0 и среднее значение координаты $\langle z\rangle$ адсорбированных атомов.

Указание. $\varphi \operatorname{ctg}\varphi = -1,21$ при $\varphi = 2\pi/3$.

3.

21. $U_0 = 4$ K, $\langle z\rangle \approx \frac{\pi}{2k} + \frac{1}{2x} \approx 7$Å.

Здесь $k = \frac{1}{\hbar}\sqrt{2m\mathscr{E}_1}; x = \frac{1}{\hbar}\sqrt{2m\left(U_0 - \mathscr{E}_1\right)} = \frac{1}{\hbar}\sqrt{2m\mathscr{E}}; \mathscr{E}_1 = U_0 - \mathscr{E}$. Расчет показывает, что $\langle z\rangle \approx 5,4$Å, т. е. «в среднем» атом находится не вне ямы, а все-таки внутри нее.

O3.1-3.22

Электрон находится в одномерной симметричной потенциальной яме размером $2a = 2$Å. Отношение волновой функции основного состояния на границе ямы к ее максимальному значению внутри ямы составляет $\alpha = 1/2$. Найти щегося в основном состоянии в одномерной яме шириной $a = 2$Åс потенциалом $U(0) = \infty, U = -U_0$ при $0 < x <$ и $U = 0$ при $x > a$, если известно, что от- ношение волновой функции на границе ямы ($x = a$) к ее максимальному значению в яме равно $\alpha = \sqrt{3}/2$.

3.

22. $U_0 = \frac{2\pi^2\hbar^2}{9ma^2} = 16,6$ эВ; $\mathscr{E} = \frac{\pi^2\hbar^2}{6ma^2} = 12,45$ эВ .

23

3.

23. $U_0 = \frac{8\pi^2\hbar^2}{27ma^2} = 5,53\ni$ В; $\mathscr{E} = \frac{U_0}{4} = 1,38$ В.

O3.1-3.24

Частица, находящаяся в потенциальной яме с бесконечно высокими стенками, излучает фотон, переходя из состояния с номером $(n + 1)$ в состояние n. Найти связь частоты фотона с периодом колебаний между стенками классической ямы частицы с энергией $\mathscr{E}_n$.

3.

24* Решение. Энергия частицы m, находящейся в одномерной потенциальной яме шириной a, квантуется

$$\mathscr{E}_n = \frac{\pi^2\hbar^2}{2ma^2}n^2$$

При переходе частицы из состояния $n+1$ в состояние n излучается квант энергии с частотой

$$\omega_{n+1,n} = \frac{\mathscr{E}_{n+1} - \mathscr{E}_n}{\hbar} = \frac{\pi^2\hbar}{2ma^2}(2n+1)$$

Классическая частица колеблется в яме с частотой $\omega_{\text{кл}} = 2\pi/T$, где $T = 2a/v$, где в свою очередь v - скорость частицы при движении от стенки к стенке - определяется ее энергией. Для сравнения примем значение энергии равным E_n. Тогда

$$v = \sqrt{\frac{2\S_n}{m}} = \frac{\pi\hbar n}{ma}; \omega_{\text{K}\Omega} = \frac{\pi v}{a} = \frac{\pi^2\hbar n}{ma^2}.$$

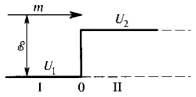
Теперь сравним $\omega_{n+1,n}$ с $\omega_{\text{кл}}$:

$$\frac{\omega_{n+1,n}}{\omega_{\text{kT}}} = 1 + \frac{1}{2n} \to 1 \quad \text{при } n \to \infty.$$

Эта задача является иллюстрацией принципа соответствия Бора. При больших значениях квантовых чисел квантово-механическое поведение системы переходит в классическое.

О3.1-3.25

Свободно движущаяся частица массой m с энергией $\mathscr{E}$ подходит к границе раздела двух областей I и II, на которой потенциальная энергия частицы скачкообразно меняется от постоянного значения U_1 до постоянного значения U_2 (рис. 26).



Определить коэффициенты отражения и пропускания частицы на этой границе по амплитуде (r и d) и по энергии (R и D). Исследовать случаи, когда: 1) $\mathscr{E} > U_2$ и 2) $\mathscr{E} < U_2$. Во втором случае определить среднюю глубину проникновения l частицы во вторую среду.

3.

25* Решение. Запишем уравнение Шредингера в виде

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \tag{1}$$

де

$$k^2 = \frac{2m}{\hbar^2}(\mathscr{S} - U) \tag{2}$$

В области I волновая функция частицы состоит из падающей волны

$$\psi_1 = e^{i(k_1x - \omega t)}$$

и отраженной

$$\psi_1' = re^{-i(k_1x + \omega t)}$$

а в области II - из прошедшей волны

$$\psi_2 = de^{i(k_2x - \omega t)}$$

где индексами 1 и 2 отмечены волновые векторы в областях I и II соответственно. Амплитуда падающей волны принята равной единице, что, очевид но, не нарушает общности получаемых ниже результатов. Волновая функция и ее производная по x на границе раздела должны быть непрерывны. Это приводит к соотношениям

$$1 + r = d, \quad k_1 - k_1 r = k_2 d$$

из которых находим

$$r = \frac{k_1 - k_2}{k_1 + k_2}, \quad d = \frac{2k_1}{k_1 + k_2}. \tag{3}$$

1. Если $\mathscr{E} > U_2$, то волна ψ_2 однородна, так же как падающая волна ψ_1 и отраженная ψ_1'. Вычислим плотности потоков вероятностей для отраженной волны

$$j_r = \frac{i\hbar}{2m}\left[\psi_1' \frac{d\psi_1'^*}{dx} - \psi_1'^* \frac{d\psi_1'}{dx}\right] = \frac{i\hbar}{2m}\left[r^2 ik_1 + r^2 ik_1\right] = -r^2 \frac{\hbar k_1}{m}$$

и для прошедшей волны

$$\dot{j}_d = \frac{i\hbar}{2m}\left[\psi_2 \frac{d\psi_2^*}{dx} - \psi_2^* \frac{d\psi_2}{dx}\right] = d^2 \frac{\hbar k_2}{m}$$

Плотность потока вероятностей для падающей волны $j_e = \hbar k_1/m = v_1$ (равна скорости частицы, налетающей на барьер). Вычислим энергетические коэффициенты отражения R и прохождения D:

$$R = \left|\frac{j_r}{j_e}\right| = \left|-r^2\right| = \left|\frac{k_1 - k_2}{k_1 + k_2}\right|^2$$
$$D = \left|\frac{j_d}{j_e}\right| = \frac{k_2}{k_1} d^2 = \frac{4k_1 k_2}{(k_1 + k_2)^2} \tag{4}$$

Величины этих коэффициентов находятся в согласии с законом сохранения энергии: $R + D = 1$.
2) Если $\mathscr{E} < U_2$, то k_2 - чисто мнимое, т. е. волна во второй области неоднородна. В этом случае $R = 1$, т. е. отражение полное. Полагая $k_2 = i\alpha$, для волны во второй области получим

$$\psi_2 = \frac{2k_1}{k_1 + k_2} e^{-\alpha x} e^{-i\omega t}, \tag{5}$$

т. е. амплитуда волны в области II экспоненциально затухает при удалении от границы раздела областей.

Глубина проникновения l определяется как расстояние, на котором плотность потока энергии убывает в e раз. Для нее получаем

$$l = \frac{1}{2}\alpha = \frac{\hbar}{2\sqrt{2m\,(U_2 - \S)}}, \tag{6}$$

О3.1-3.26 Отражения от ямы (???)

Электрон, находящийся в одномерной прямоугольной потенциальной яме шириной несколько сантиметров и глубиной несколько электрон-вольт, поглощает квант света с частотой $v = 1,01 v_0$, где v_0 - предельная частота света, при которой электрон может вылететь из ямы. Определить среднее число отражений N от краев ямы, которые испытывает электрон, прежде чем покинуть ее. Считать, что время радиационного перехода электрона в основное состояние много больше времени вылета электрона из ямы.

3.

26. $N \approx \frac{1}{D} \approx \frac{1}{4}\sqrt{\frac{v_0}{\nu - v_0}} = 2,5$, где D - коэффициент прохождения.

Примечание. Видно, что число ударов очень мало, т. е. здесь состояние «слабо стационарное», и обычно используемое выражение для числа ударов через коэффициент отражения плоской волны от барьера в данном случае является очень грубой оценкой, дающей представление лишь о порядке величины числа отражений.

О3.1-3.27

Электрон, находящийся в основном состоянии в одномерной потенциальной яме шириной $a = 4$ Åи глубиной $U_0 = 10$ эВ (рис. 27) переведен в возбужденное состояние с энергией $\approx 10^{-2}$ эВ (нуль отсчета энергии - состояние покоя вне ямы). Оценить время жизни возбужденного состояния, считая, что оно ограничивается вылетом электрона из ямы, а не переходом в основное состояние.

3.

27. $\tau \approx (nD)^{-1} \approx \frac{a}{4}\sqrt{\frac{m}{2\delta}} \sim 10^{-15}$ с, где $n = \frac{1}{a}\sqrt{\frac{2U_0}{m}}$ - частота ударов о стенки ямы; $D = 4\frac{\sqrt{\mathscr{E}(U_0+\mathscr{E})}}{\left(\sqrt{U_0+\mathscr{E}}+\sqrt{\mathfrak{E}}\right)^2} \approx 4\sqrt{\frac{\mathscr{E}}{U_0}}$ - коэффициент прохождения. См. также примечание к ответу предыдущей задачи.

O3.1-3.28

Электрон, введенный в жидкий гелий, расталкивает атомы жидкости и образует в ней сферическую вакуумную полость, которая является для электрона потенциальной ямой с практически бесконечно высокой стенкой. Вычислить радиус полости, если поверхностное натяжение жидкого гелия равно 0,35 дин/см, а электрон занимает в полости наинизший квантовый уровень. Внешнее давление считать равным нулю.

3.

28. $R = \sqrt[4]{\frac{\pi\hbar^2}{8\sigma m}} \approx 20$Å, см. также решение задачи 3.16 .

O3.1-3.29-46 THEY ARE MISSING, I'LL ADD LATER

SOLUTIONS 3. Уравнение Шредингера. Квантование. Потенциальные барьеры.

3.

29. $l = 0,56$НМ.

3.

30. Решение. В области I $(x < 0)$ $\psi_I = e^{ik_1 x} + re^{-ik_1 x}$, где $k_1^2 = 2m\left(\mathscr{E} - U_1/\hbar^2\right.$. В области барьера $(0 < x < l)\psi = ae^{ikx} + be^{-ikx}$, где $k^2 = 2m(\mathscr{E} - U)/\hbar^2$. В области $II(x > l)\psi_{II} = de^{ik_2 x}$, где $k_2^2 = 2m\left(\mathscr{E} - U_2\right)/\hbar^2$.

Сшивая волновые функции и их производные в точках $x = 0$ и $x = l$, получим систему уравнений относительно r, d, a и b:

$$\begin{array}{ll} 1 + r = a + b; & ae^{ikl} + be^{-ikl} = de^{ik_2 l}; \\ k_1 - k_1 r = ka - kb; & kae^{ikl} - kbe^{-ikl} = k_2 de^{ik_2 l}. \end{array}$$

Отсюда получаем

$$r = \frac{\left(k_1 - k\right)\left(k + k_2\right) + \left(k_1 + k\right)\left(k - k_2\right)e^{2ikl}}{\left(k_1 + k\right)\left(k + k_2\right) + \left(k_1 - k\right)\left(k - k_2\right)e^{2ikl}},$$

$$d = \frac{4k_1 k e^{-ii(k_2 - k)l}}{\left(k_1 + k\right)\left(k + k_2\right) + \left(k_1 - k\right)\left(k - k_2\right)e^{2ikl}}.$$

В случае, когда энергия частицы ниже высоты барьера, т.е. $\mathscr{E} < U$, волновая функция в области барьера имеет вид $\psi = ae^{-xx} + be^{xx}$, где $x^2 = 2m(U - \S)/\hbar^2$, и в этом случае в формулах для r и d нужно провести замену $k \to ix$. Таким образом, поскольку в области II мы по-прежнему имеем прошедшую плоскую волну, то получаем важный вывод - квантово-механическая частица может проходить сквозь барьер даже в том случае, когда ее энергия меньше высоты барьера («туннельный эффект»).

3.

31. Полная энергия $\mathscr{E}$ должна быть больше потенциальной энергии U частицы внутри барьера (ямы). Толщина барьера (ямы) должна быть $l = \lambda/2, \lambda, 3\lambda/2, 2\lambda, 5\lambda/2, ...$, где $\lambda = h/\sqrt{2m(\mathscr{E} - U)}$ - длина волны де Бройля частицы в области барьера (ямы), или, иначе, $l = \pi\hbar p/\sqrt{2m(\mathscr{E} - U)}$ и одновременно

$\mathscr{E} = U + \frac{\pi^2\hbar^2}{2ml^2}p^2$, где $p = 1, 2, ...$, т. е. энергия частицы должна совпадать с одним из собственных значений энергии в бесконечно глубокой потенциальной яме, дно которой расположено на высоте барьера.

3.

32. $\mathscr{E}_n = U + \frac{\pi^2\hbar^2}{2ml^2}n^2, \quad n = 1, 2, 3, ..., \quad$ или в числах $\quad \mathscr{E}_n = \left(5 + 37,62n^2\right)$ эВ.

3.

33. $R \approx \frac{h}{4\sqrt{2m(\text{Å}+U)}} \approx 1,7$Å. (Табличное значение $R = 1,98$Å).

3.

34. $U = \frac{\mathscr{E}}{\sin^2 kd} = 1,64$ эВ, где $k = \frac{1}{\hbar}\sqrt{2m\mathscr{E}} = 6,22 \cdot 10^7$ см$^{-1}$. $D \approx \exp(-18xd) \approx 3,2 \cdot 10^{-5}$, где $x = \frac{1}{\hbar}\sqrt{2m(U-\mathcal{E})} \approx 1,9 \cdot 10^7$ см$^{-1}$; $\tau = \frac{\ln 2}{nD} \approx 1,8 \cdot 10^{-11}$с, где $n = \frac{1}{2d}\sqrt{\frac{2}{m}} \approx 1,22 \cdot 10^{15}$с$^{-1}$.

3.

35. $\tau = \frac{1}{nD} \approx 1,2 \cdot 10^{-11}$с, где $D \approx \exp(-598ax) \approx 8,3 \cdot 10^{-5}$, $x = \sqrt{2m(U-\mathscr{E})}/\hbar \approx 5,08 \cdot 10^5$ см$^{-1}$, $a = 3$Å.

3.

36: Решение. На рис. 151 обозначен подбарьерный переход α-частицы с энергией $\mathfrak{E}$. Так как заряд α-частицы $Z_\alpha = 2$, то оставшаяся часть ядра имеет заряд $Z' = Z - Z_\alpha = Z - 2$. $U(r) = Z'Z_\alpha e^{2/r}$. По условию $\mathscr{E} \ll U(R)$. Вычислим коэффициент прозрачности барьера по известной формуле

$$D \approx \exp\left\{-\frac{2}{\hbar}\int_R^{R_1}\sqrt{2m\left(\frac{z'z_a e^2}{r} - \delta\right)}dr\right\}$$

В подынтегральном выражении можно пренебречь $\mathscr{E}$ в силу указанного в условии неравенства. Вычислим этот интеграл

$$I = -\frac{2}{\hbar}\int_R^{R_1}\sqrt{2m\frac{Z'Z_\alpha e^2}{r}}dr = -\frac{2}{\hbar}\sqrt{2mZ'Z_\alpha e^2}\int_R^{R_1} r^{-1/2}dr =$$
$$= -\frac{4}{\hbar}\sqrt{2mZ'Z_\alpha e^2 R_1}\left(1 - \sqrt{\frac{R_1}{R}}\right)$$

Из рис. 151 видно, что $\frac{Z'Z_\alpha e^2}{R_1} = \mathscr{E}$, откуда $R_1 = \frac{Z'Z_\alpha e^2}{\mathscr{E}}$.

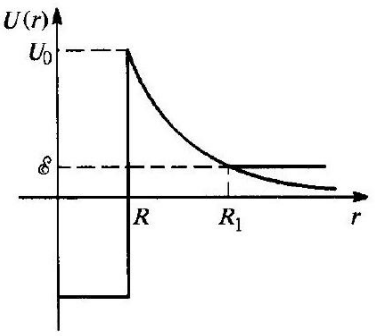


Рис. 151
Подставляя это в формулу для I, получаем

$$I \approx -\frac{4}{\hbar} Z' Z_\alpha e^2 \sqrt{\frac{2m}{\varrho}}$$

где использовано очевидное неравенство $R_1 \gg R$, справедливое в силу заданного условия $\mathscr{E} \ll U(R)$. Таким образом,

$$D \approx \exp\left(-\frac{4}{\hbar} Z' Z_\alpha e^2 \sqrt{\frac{2m}{\mathscr{E}}}\right) = \exp\left(-\frac{A}{\sqrt{\mathfrak{G}}}\right)$$

Для приближенной оценки вероятности распада в единицу времени (постоянной распада) λ необходимо прежде всего оценить число столкновений α-частицы с потенциальной стенкой за 1с : $n \approx v/(2R)$, где v - скорость α-частицы внутри ядра, которую оценим из соотношения неопределенностей:

$$v = \frac{p}{m_a} \approx \frac{\hbar}{m_a R}; \quad n \approx \frac{v}{2R} \approx \frac{\hbar}{2m_a R^2}$$

Вероятность распада в единицу времени

$$\lambda \approx nD \approx \frac{\hbar D}{2m_a R^2}$$

Период полураспада T ядра, как известно, равен

$$T = \frac{\ln 2}{\lambda} \approx \frac{2m_a R^2 \ln 2}{\hbar D} \approx a \exp\left(-\frac{b}{\sqrt{6}}\right)$$

где a и b - очевидные константы. Прологарифмировав это выражение, получим закон Гейгера-Неттола

$$\lg T \approx A + \frac{B}{\sqrt{6}}$$

3.

37* Р ешение.

Оценка изменения туннельного тока может быть проведена при рассмотрении одномерной задачи (рис. 152).

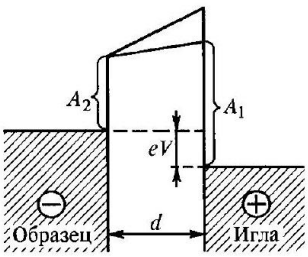


Рис. 152

Обратим внимание, что на такой энергетической диаграмме потенциальная энергия электронов возрастает снизу вверх, а потенциал поля - наоборот.

Очевидно, что туннельный ток пропорционален прозрачности барьера, изображенного на рис. 152.

$$D = D_0 \exp\left[-\frac{2}{\hbar}\int_0^d \sqrt{2m\left(A_2 + eEx\right)}dx\right]$$

где напряженность электрического поля $E = \left(A_1 - A_2 - eV\right)/d$. Интеграл в показателе экспоненты легко вычисляется:

$$\frac{2}{\hbar}\int_0^d \sqrt{2m\left(A_2 + eEx\right)}dx = \frac{4}{3\hbar}\frac{\sqrt{2m}}{eE}\left[\left(A_2 + eEd\right)^{3/2} - A_2^{3/2}\right]$$

Следовательно, прозрачность барьера

$$D = D_0 \exp\left\{-\frac{4}{3\hbar}\frac{\sqrt{2m}d}{\left(A_1 - A_2 - eV\right)}\left[\left(A_1 - eV\right)^{3/2} - A_2^{3/2}\right]\right\}$$

При перемещении иглы над ступенькой высотой b в полученном выражении следует заменить d на $d - b$. Таким образом, ток возрастет в

$$\frac{\mathscr{J}(d-b)}{(d)} = \exp\left\{\frac{4\sqrt{2m}}{3\hbar(A_1 - A_2 - eV)}\left[(A_1 - eV)^{3/2} - A_2^{3/2}\right]b\right\} = e^{2,08} \approx 8 \text{ раз.}$$

3.

38. Ток уменьшится: $\frac{\mathfrak{g}'}{\mathfrak{r}} = e^{-0,82} \approx 0,44$.

3.

39. $\delta_{\mathscr{E}} = 0,27$НА.

3.

40. $D \approx \exp\left(-\frac{4e}{\hbar}\sqrt{2\mu R_2}\right) \approx e^{-234,7} \approx 10^{-102}$, где $\mu = \frac{m_{\text{D}}}{2} = m_{\text{p}}$ - приведенная масса системы из двух дейтронов.

3.

41. $D \approx \exp\left(-\frac{\pi a\sqrt{2m}(U_0-\mathscr{E})}{\hbar\sqrt{U_0}}\right) = \exp\left(-2\pi\frac{U_0-\mathscr{E}}{\hbar\omega}\right)$, где $\mathscr{E}$ - энергия возбуждения ядра, a - координата классической точки поворота.

3.

42. $f = \left|\frac{A_1}{A_2}\right|^2 = \frac{1}{1+(U_0/\mathscr{E})\cos^2 k_1 a}$, где $k_1^2 = \frac{2m}{\hbar^2}(\mathscr{E} + U_0), A_1$ - максимальное значение ψ-функции в области $0 < x \leqslant a; A_2$ - в области $a \leqslant x < b$.

При $U_0 \gg \mathscr{E}$ величина $f \to 0$ при всех $\mathscr{E}$, кроме «резонансных» значений (когда $\cos k_1 a = 0$). При этом $\mathscr{E}_n = \frac{(2n+1)^2\pi^2\hbar^2}{8ma^2} - U_0, n = 0, 1, 2, ...$, а $f = 1$.

3.

43* Решение. Атом гелия участвует во вращательном движении. Момент импульса этого движения квантуется

$$m_{\text{He}}{}^{vr} = n\hbar, \quad n = 1, 2, 3, ...$$

По условию, если v - скорость атомов гелия в вихре, то $vr = K$ - интенсивность вихря. Откуда

$$K = \frac{\hbar}{m_{\text{He}}}n; K_{\min} = \frac{\hbar}{m_{\text{He}}} = 1,6 \cdot 10^{-4} \text{ см}^2/\text{с}$$

3.

44. $v(r) = \frac{n\hbar}{m_{\text{He}}r}$.

3.

45. $L_{\min} = \lambda/4$.

3.

46. $L_{\min} = \lambda/4$.

3.

47. Энергия связи $\mathscr{E} = \frac{\hbar^2\alpha^2}{8ma^2} = 3,8 \cdot 10^{-4}$ В, $U - \mathscr{E} = \frac{\hbar^2\alpha}{4ma^2} = 7,63 \cdot 10^{-3}$ эВ. Глубина потенциальной ямы $U = (U - \mathscr{E}) + \mathscr{E} = \frac{\hbar^2}{4ma^2}\left(\alpha + \frac{\alpha^2}{2}\right) = 8 \cdot 10^{-3}$ В.

3.

48. $\mathscr{E}_{CB} = U_0 - \mathscr{E} = \frac{\hbar^2\alpha^2}{2ma^2} = 123\kappa$ В.

3.

49. $\frac{a}{a'} = \frac{8}{3\sqrt{3}} \approx 1,54$, где a' - ширина «сжатой» ямы.

3.

50. $\frac{U_0}{U_0'} = \frac{9}{2} = 4,5$, где U_0' - измененная высота ямы.

17.3.6 Problems about basic 1D scatterings 3

О3.1-3.47. Свойства электрона в яме

Электрон находится в основном состоянии в одномерной симметричной прямоугольной потенциальной яме **с** шириной $2a = 10$Åс потенциалом $U(\pm\infty) = 0$. Отношение вероятностей обнаружить частицу внутри и вне ямы равно $\alpha = 0,1$. Считая, что изменение волновой функции внутри ямы мало, определить энергию связи электрона и глубину ямы (в эВ).

Solution.

(! решу заново!)
решаем графически равенство:

$$|\cos ka| = \gamma ka$$

подставляем условие задачи:

$$\frac{w_1}{w_2} = \alpha = \frac{2a}{\frac{A^2}{2\kappa}e^{-2\kappa a}}$$

О3.1-3.48

Нейтрон находится в основном состоянии в одномерной прямоугольной потенциальной яме с шириной $a = 1,3{\cdot}10^{-13}$ cm, ограниченной с одной стороны бесконечно высокой стенкой. При этом $U = 0$ при $0 < x < a$, а при $x \geqslant a$ потенциал U равен постоянной конечной величине U_0. Отношение вероятностей обнаружить частицу внутри и вне ямы равно $\alpha = 0,1$. Считая, что максимум волновой функции достигается вблизи границы ямы, определить энергию связи нейтрона.

Solution.

(?? см выше решения, по идее уже метод для этой задачи обсуждался)

3.48. $\mathscr{E}_{\text{СВ}} = U_0 - \mathscr{E} = \frac{\hbar^2\alpha^2}{2ma^2} = 123$ кэВ.

О3.1-3.49. Сжатие ямы

Микрочастица находится в прямоугольной потенциальной яме заданной ширины. Одна стенка бесконечная, а вторая - конечная, высотой U_0. Энергия частицы в яме $\mathscr{E} = 3U_0/4$. Во сколько раз надо квазистатически «сжать» яму при неизменной высоте, чтобы частица стала свободной?

Solution.

Пишем УШ для этого случая, в двух областях:

$$\phi'' + k^2\psi = 0$$
$$\phi'' + \kappa^2\psi = 0,$$

где $k^2 = 2mE/\hbar^2, \kappa^2 = k = 2m(U_0 - E)/\hbar^2$.

Сшивка решений:

$$A\sin ka = Be^{-\kappa a}$$
$$Ak\cos ka = -B\kappa e^{-\kappa a}$$

В итоге:

$$\cot ka = -\frac{\kappa}{k}$$

Распишем

$$\cot^2 ka = -\frac{\kappa^2}{k^2} = \frac{U_0}{E} - 1,$$

отсюда, переходя к синусу по $\cot^2 x + 1 = \sin^{-2} x$, получаем, подставив $E = \hbar^2k^2/2m$

$$|\sin ka| = \sqrt{\frac{\hbar^2k^2}{2mU_0}\cdot\frac{a^2}{a^2}} \equiv \gamma ka,$$

где $\gamma = \sqrt{\frac{\hbar^2}{2mU_0a^2}}$

(?? ничего, что $\gamma = \gamma(a)$???)

(дальше рисуем графически!!)

(вроде уже решал такую задачу, где граф метод, вроде точно для такой же задачи)

Первый уровень появляется при $ka = \pi/2$ (??? имеется в виду, что E это не из условий, а в зависимости от ширины ямы) $U_0 = E$. То есть $\gamma = 22/pi^2$, откуда условие первого уровня:

$$U_0a^2 = \frac{\pi^2\hbar^2}{8m},$$

В нашей задаче при данных энергиях, находим из контангенса

$$ka = \frac{2\pi}{3},$$

подставим $a = a(U_0)$, получим

$$U_0a^2 = \frac{8\pi^2\hbar^2}{27m}$$

(??? это было до сжатия??)

(теперь пишем после сжатия)

В итоге

$$\frac{a}{a_{\text{конечн}}} = \frac{8}{3\sqrt{3}}$$

(паререшаю потом сам!!!.)

Ответ: 3.49. $\frac{a}{a'} = \frac{8}{3\sqrt{3}} \approx 1,54$, где a' - ширина «сжатой» ямы.

О3.1-3.50

Микрочастица находится в одномерной потенциальной яме заданной ширины. Одна ее стенка бесконечно высокая, а вторая конечной высоты U_0. Энергия частицы в яме $\mathscr{E} = U_0/2$. Во сколько раз надо квазистатически изменить высоту ямы при неизменной ширине, чтобы частица стала свободной?

Solution.

(?? см выше решения, по идее уже метод для этой задачи обсуждался)

3.50. $\frac{U_0}{U_0'} = \frac{9}{2} = 4,5$, где U_0' - измененная высота ямы.

О3.1-3.51

Электрон находится в одномерной прямоугольной потенциальной яме с шириной $a = 4$ Å$(U(0) = \infty, U(a) = U_0 = 1$ эВ) в состоянии с энергией $\mathscr{E} = 0,88$ эВ. На яму накладывается постоянное электрическое поле $E = 3 \cdot 10^5$ В/см, направленное в отрицательную сторону оси x. Оценить возникающую при этом ширину уровня энергии. Считать, что энергия уровня не меняется при наложении поля.

3.

51. $\Gamma \simeq \frac{\hbar D}{2a}\sqrt{\frac{2\varepsilon}{m}} = 3,6 \cdot 10^{-5}$эВ, где проницаемость возникающего барьера треугольной формы (рис. 153).

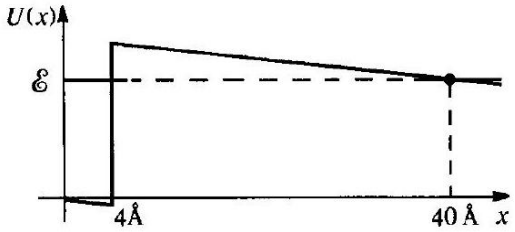


Рис. 153

$D \simeq \exp\left[-\frac{4}{3}\frac{\sqrt{2m(U_0-\mathscr{E})}}{\hbar eE}(U_0-\mathscr{E})\right] \simeq \simeq 7,8 \cdot 10^{-5}$.

Параметры задачи подобраны так, что в яме есть только один уровень: $\sin ka = \sqrt{\frac{\hbar^2}{2mU_0a^2}}ka = 0,488ka$, откуда $ka = 1,92$. Величина $eEa = 0,012$ эВ $\ll U_0 - \delta = 0,12$ эВ.

О3.1-3.52

Электрон находится в одномерной симметричной прямоугольной потенциальной яме с шириной $2a =$ 4 Å$(U(-a) = U(a) = U_0 = 1$ эВ) в состоянии, энергия которого $\mathscr{E} = 0,8$ эВ. На яму накладывается постоянное электрическое поле $E = 3 \cdot 10^5$ В/см, направленное в отрицательную сторону оси x. Оценить время, через которое электрон покинет яму. Считать, что энергия уровня не меняется при наложении поля.

3.

52. $\tau \simeq \frac{4a}{vD} = \frac{4a}{D}\sqrt{\frac{m}{2\S}} \simeq 10^{-6}$ с, где проницаемость возникающего барьера треугольной формы $D \simeq \exp\left[-\frac{4}{3}\frac{\sqrt{2m(U_0-\mathscr{E})}}{\hbar eE}(U_0-\mathscr{E})\right] \simeq 1,45 \cdot 10^{-9}$.

Параметры задачи подобраны так, что в яме есть только один четный уровень: $\cos ka = \sqrt{\frac{\hbar^2}{2mU_0a^2}}ka = 1,94ka$, откуда $ka = 0,46$.

17.3.7 Problems about scattering in Born approximation 1

В этом разделе задачи, которые важно прорешать для понимания рассеяния.

Б-2.12.2 Рассеяние в рамках правила Ферми

С помощью «золотого правила Ферми» получить формулу для дифференциального сечения рассеяния в борновском приближении.

Solution.

(по теории, пропишу скоро)

Б-2.12.3 Формулы для δ_l в борновском приближении (!!!)

Определить фазы рассеяния δ_l в борновском приближении.

Solution.

(по теории, пропишу скоро)

Б-2.12.4 Рассеяние в $1/r^2$

Для модельного потенциала отталкивания

$$V(r) = \frac{\beta}{r^2}, \quad \beta > 0$$

найти фазы рассеяния δ_l. В предельном случае $2m\beta/\hbar^2 \ll 1$ найти приближенное выражение для фаз $\delta_l \ll 1$, и, выполнив суммирование ряда разложения амплитуды рассеяния по парциальным волнам, получить замкнутое выражение для амплитуды $f(\theta)$. Сравнить полученное выражение с борновским приближением.

Solution.

Б-2.12.5 Свойство рассеяния медленных частиц

Показать, что при рассеянии медленных частиц на потенциале с малым радиусом действия a наиболее существенную роль играет рассеяние s-волн ($l = 0$).

Solution.

(по теории, пропишу скоро)

Б-2.12.6 Аппроксимация δ-потенциалом

Показать, что при рассеянии медленной частицы массы m, рассеивающий потенциал может быть заменен контактным псевдопотенциалом

$$V_{\text{eff}} = -\frac{2\pi\hbar^2}{m} a\delta(\mathbf{r}),$$

где a - длина рассеяния (радиус действия потенциала). Данное выражение часто используется для описания рассеяния медленных нейтронов ядрами.

Solution.

GKKG.13.1.a Basic model for Born approximation

Using the Born approximation, find the scattering amplitude and the total scattering cross-section of a particle on the following potentials:

a) $U(r) = \frac{\alpha}{r} e^{-r/R}$

Consider the limiting cases of slow and fast particles. Find the conditions under which the approximations in these limiting cases are valid.

a)

So, we need to just use:

$$f_{3D}^{B}(q) = -\frac{2m}{\hbar^2 q}\int\limits_0^\infty U(r)\sin(qr)rdr \tag{XIII.8}$$

$$\sigma(E) = \int |f|^2 d\Omega = 2\pi\int\limits_0^\pi |f|^2\sin\theta d\theta = \frac{\pi\hbar^2}{2mE}\int\limits_0^{8mE/\hbar^2} f^2(q)dq^2, \tag{1}$$

$q := 2k\sin(\theta/2)$.

$f = -\frac{2m\alpha R^2}{\hbar^2(1+q^2R^2)}$, $\quad \sigma(E) = 16\pi\left(\frac{m\alpha R^2}{\hbar^2}\right)^2\frac{1}{1+4k^2R^2}$.

The first integral here is taken by evaluating integral with $\sin(qr) \to e^{iqr}$ and then by taking imaginary part. The second integral is easy, just one needs to substitute $k = \sqrt{1me/\hbar}$ in the end.

For R finite, the scattering cross-section also has a finite magnitude. However, as $R \to \infty$, the short-range Yukawa potential considered here changes to a long-range Coulomb potential $U = \alpha/r$. For the latter, the differential cross-section is described by the Rutherford formula, $d\sigma/d\Omega = 4m^2\alpha^2/\hbar^4q^4$, and the total scattering cross-section is infinite.

GKKG.13.b Basic model for Born approximation

Using the Born approximation, find the scattering amplitude and the total scattering cross-section of a particle on the following potentials:

b) $U(r) = \alpha\delta(r - R)$;

b)

So, we need to just use:

$$f_{3D}^{B}(q) = -\frac{2m}{\hbar^2 q}\int\limits_0^\infty U(r)\sin(qr)rdr \tag{XIII.8}$$

$$\sigma(E) = \int |f|^2 d\Omega = 2\pi\int\limits_0^\pi |f|^2\sin\theta d\theta = \frac{\pi\hbar^2}{2mE}\int\limits_0^{8mE/\hbar^2} f^2(q)dq^2, \tag{1}$$

$q := 2k\sin(\theta/2)$.

$f = -\frac{2m\alpha R^2}{\hbar^2}\frac{\sin qR}{qR}$, $\qquad \sigma(E) = \frac{4\pi m\alpha^2R^2}{\hbar^2E}\int\limits_0^{\sqrt{8mER^2/\hbar^2}}\frac{\sin^2 x}{x}dx$.

It is obvious how to obtain both integrals.

In the limiting cases, we have

$$\sigma(E)E \underset{\approx}{\to} 0\frac{16\pi\left(m\alpha R^2\right)^2}{\hbar^4}, \quad \sigma(E)E \underset{\approx}{\to} \infty\frac{\pi m\alpha^2R^2}{\hbar^2E}\ln\frac{8mER^2}{\hbar^2}$$

In the $E \to \infty$ limit, the integral in (3) diverges; to calculate this diverging integral we replace the oscillating factor $\sin^2 x$ by its mean value, 1/2.

GKKG.13.1.c Basic model for Born approximation

Using the Born approximation, find the scattering amplitude and the total scattering cross-section of a particle on the following potentials:

c) $U(r) = U_0e^{-r/R}$

Consider the limiting cases of slow and fast particles. Find the conditions under which the approximations in these limiting cases are valid.

c)

So, we need to just use:

$$f_{3D}^{B}(q) = -\frac{2m}{\hbar^2 q}\int\limits_0^\infty U(r)\sin(qr)rdr \tag{XIII.8}$$

$$\sigma(E) = \int |f|^2 d\Omega = 2\pi\int\limits_0^\pi |f|^2 \sin\theta d\theta = \frac{\pi\hbar^2}{2mE}\int\limits_0^{8mE/\hbar^2} f^2(q)dq^2, \tag{1}$$

$q := 2k\sin(\theta/2)$.

$f = -\frac{4mU_0R^3}{\hbar^2(1+q^2R^2)^2}$; $\sigma(E) = \frac{8\pi mR^4U_0^2}{3\hbar^3E}\left[1 - \frac{1}{(1+8mER^2/\hbar^2)^3}\right]$

The first integral is taken by $\sin(qr) \to e^{iqr}$, integration by parts and then by taking imaginary part.

GKKG.13.1.d Basic model for Born approximation

Using the Born approximation, find the scattering amplitude and the total scattering cross-section of a particle on the following potentials:

d) $U(r) = \frac{\alpha}{r^2}$

Consider the limiting cases of slow and fast particles. Find the conditions under which the approximations in these limiting cases are valid.

d)

So, we need to just use:

$$f_{3D}^{B}(q) = -\frac{2m}{\hbar^2 q}\int\limits_0^\infty U(r)\sin(qr)rdr \tag{XIII.8}$$

$$\sigma(E) = \int |f|^2 d\Omega = 2\pi\int\limits_0^\pi |f|^2 \sin\theta d\theta = \frac{\pi\hbar^2}{2mE}\int\limits_0^{8mE/\hbar^2} f^2(q)dq^2, \tag{1}$$

$q := 2k\sin(\theta/2)$.

$f = -\frac{\pi m\alpha}{\hbar^2 q} = -\frac{\pi m\alpha}{2\hbar^2 k\sin(\theta/2)}$.

The integral is just an "integral sine".

The total scattering cross-section is infinite, which is related to a slow decrease of the potential at large distances. For more on scattering from the potential $U = \alpha/r^2$, see Problem 13.19.

GKKG.13.1.e Basic model for Born approximation

Using the Born approximation, find the scattering amplitude and the total scattering cross-section of a particle on the following potentials:

e) $U(r) = \begin{cases} U_0, r < R \\ 0, \quad r > R \end{cases}$

Consider the limiting cases of slow and fast particles. Find the conditions under which the approximations in these limiting cases are valid.

e)

So, we need to just use:

$$f_{3D}^{B}(q) = -\frac{2m}{\hbar^2 q}\int\limits_0^\infty U(r)\sin(qr)rdr \tag{XIII.8}$$

$$\sigma(E) = \int |f|^2 d\Omega = 2\pi\int\limits_0^\pi |f|^2 \sin\theta d\theta = \frac{\pi\hbar^2}{2mE}\int\limits_0^{8mE/\hbar^2} f^2(q)dq^2, \tag{1}$$

$q := 2k\sin(\theta/2)$.

$f = \frac{2mU_0R}{\hbar^2q^2}\left(\cos qR - \frac{\sin qR}{qR}\right)$; $\quad \sigma(E) = \frac{2\pi}{k^2}\left(\frac{mU_0R^2}{\hbar^2}\right)^2\left[1 - \frac{1}{(2kR)^2} + \frac{\sin 4kR}{(2kR)^3} - \frac{\sin^2 2kR}{(2kR)^4}\right]$.

The first integral is evaluated by parts, the second is obvious.

In the limiting cases we have

$$\sigma(E)E \underset{\approx}{\to} 0\frac{16\pi m^2U_0^2R^6}{9\hbar^4}, \quad \sigma(E)E \underset{\approx}{\to} \infty\frac{\pi mU_0^2R^4}{\hbar^2E}$$

The limit $E \to \infty$ is also discussed in Problem 13.2.

GKKG.13.1.f Basic model for Born approximation

Using the Born approximation, find the scattering amplitude and the total scattering cross-section of a particle on the following potentials:

f) $U(r) = U_0e^{-r^2/R^2}$

Consider the limiting cases of slow and fast particles. Find the conditions under which the approximations in these limiting cases are valid.

f)

So, we need to just use:

$$f^B_{3D}(q) = -\frac{2m}{\hbar^2q}\int\limits_0^\infty U(r)\sin(qr)rdr \tag{XIII.8}$$

$$\sigma(E) = \int |f|^2d\Omega = 2\pi\int\limits_0^\pi |f|^2\sin\theta d\theta = \frac{\pi\hbar^2}{2mE}\int\limits_0^{8mE/\hbar^2} f^2(q)dq^2, \tag{1}$$

$q := 2k\sin(\theta/2)$.

$f = -\frac{\sqrt{\pi}mU_0R^3}{2\hbar^2}e^{-q^2R^2/4}$ $\quad \sigma(E) = \frac{\pi^2mU_0^2R^4}{4\hbar^2E}\left(1 - e^{-4mER^2/\hbar^2}\right)$

The first integral is evaluated as follows:

$$V_{\boldsymbol{q}} = V_0\int d\boldsymbol{r}e^{-r^2/a^2 + i\boldsymbol{qr}} = V_0\int d\boldsymbol{r}e^{-\frac{1}{a^2}\left(\boldsymbol{r} - i\boldsymbol{q}a^2/2\right)^2 - q^2a^2/4} = \pi^{3/2}V_0a^3e^{-q^2a^2/4}$$

(by $\int\limits_0^\infty x^2\mathrm{e}^{-\gamma x^2}dx = \frac{1}{4\gamma}\sqrt{\frac{\pi}{\gamma}}$), here $q^2 = 4k^2\sin^2\frac{\theta}{2} = 2k^2(1 - \cos\theta)$;

$$f(\theta) = -\frac{\sqrt{\pi}}{2}V_0ma^3e^{-q^2a^2/4} = -\frac{\sqrt{\pi}}{2}V_0ma^3e^{-k^2a^2(1-\cos\theta)/2}$$

(??? я не понял пока, если мы возьмем $\sin(qr) \to e^{iqr}$ тогда у нас интеграл станет точно каким и был выше, дальше что делать? если так его сразу посчитать, то он вещественный и обратно если взять мнимую часть, получим нуль. Видимо, правильно еще сместить начало отсчета по r, тогда после этой замены от r^2 под интегралом появятся 3 интеграла, по идее они дадут такой же результат, но я не уверен в этом методе. Пока что решение очень компактно, потому что в векторных обозначениях абсолютно очевидно, что можно просто сдвинуть начало координет и избавиться от мнимой части. Другим способом - не понимаю пока, но и не важно, один способ ведь работает.)

Now, the second integral is obtained by:

$\sin\theta d\theta = d(1 - \cos\theta) = \frac{d\left(q^2\right)}{2k^2}$,

$$\sigma = \frac{\pi^2}{4}\frac{m^2a^6V_0^2}{k^2}\int\limits_0^{4k^2} d\left(q^2\right)e^{-q^2a^2/4} = \frac{\pi^2m^2a^4V_0^2}{k^2}\left(1 - e^{-k^2a^2}\right)$$

(??? тоже пока не додумал, у Галицкого 4 в знаменателе есть, по решению ПТФ - нет. где-то в одном из решений ошибка, скорее всего у ПТФ, нужно будет - найду.)

$\sigma_{\text{slow}} \approx \left(\frac{\pi V_0}{1/ma^2}\right)^2a^2 \ll a^2$; $\quad \sigma_{\text{fast}} \approx \left(\frac{\pi V_0}{1/ma^2}\right)^2\frac{1}{k^2} \ll \sigma_{\text{slow}}$ (тут опущена $\hbar$).

Due to the exponential decrease of $f(q)$, the Born approximation is not applicable for large values of q^2 (see Problem 13.13). Therefore, the inclusion of the exponentially small term in the equation for $\sigma(E)$ for $E \to \infty$ is beyond the accuracy of the approximation used.

ПТФ-13.y1.a Basic model for Born approximation

В рамках Борновского приближения, рассмотрите рассеяние на следующих потенциалах:
• $V(\mathbf{r}) = V_0 \frac{a^n}{r^n + a^n}$, $n > 3$, случай медленных частиц $ka \ll 1$. Рассмотрите также предел $n \to \infty$, когда потенциал превращается в сферическую прямоугольную яму.

Решнеие для $V(\mathbf{r}) = V_0 \frac{a^n}{r^n + a^n}$.

$$f(\theta) = -\frac{2ma^n V_0}{2k\hbar^2 \sin\frac{\theta}{2}} \int\limits_0^\infty dr \frac{r \sin\left(2kr \sin\frac{\theta}{2}\right)}{r^n + a^n} \approx -\frac{2ma^n V_0}{2k\hbar^2 \sin\frac{\theta}{2}} \int\limits_0^\infty dr \frac{2kr^2 \sin\frac{\theta}{2}}{r^n + a^n} = -\frac{2\pi m a^3 V_0}{\hbar^2 n \sin\frac{3\pi}{n}}$$

$$\sigma = 2\pi \int\limits_0^\pi |f(\theta)|^2 \sin\theta d\theta = \frac{16\pi^3 m^2 a^6 V_0^2}{\hbar^4 n^2 \sin^2\frac{3\pi}{n}}$$

При $n \to \infty$ (сферическая прямоугольная яма):

$$f(\theta) = -\frac{2ma^3 V_0}{3\hbar^2} \qquad \Rightarrow \qquad \sigma = \frac{16\pi m^2 a^6 V_0^2}{9\hbar^4}$$

ПТФ-13.y1.b Basic model for Born approximation

В рамках Борновского приближения, рассмотрите рассеяние на следующих потенциалах:
• $V(\mathbf{r}) = \frac{\alpha}{r} e^{-\kappa r}$ (потенциал Юкавы). Рассмотрите также предельный переход $\kappa \to 0$ (закон Кулона).

Решнеие для потенциала Юкавы: $V(\mathbf{r}) = \frac{\alpha}{r} e^{-\kappa r}$.

$$f(\theta) = -\frac{2m\alpha}{2k\hbar^2 \sin\frac{\theta}{2}} \int\limits_0^\infty dr \sin\left(2kr \sin\frac{\theta}{2}\right) e^{-\kappa r} = -\frac{2m\alpha}{\hbar^2 (4k^2 \sin^2\frac{\theta}{2} + \kappa^2)}$$

because $\int\limits_0^\infty e^{-\lambda r} \sin(qr) dr = \frac{1}{2i}\left[\int\limits_0^\infty e^{-(\lambda - iq)r} dr - \int\limits_0^\infty e^{-(\lambda + iq)r} dr\right]$

$$\sigma = 2\pi \int\limits_0^\pi |f(\theta)|^2 \sin\theta d\theta = \frac{8\pi m^2 \alpha^2}{\hbar^4} \int\limits_0^\pi \frac{\sin\theta d\theta}{(4k^2 \sin^2\frac{\theta}{2} + \kappa^2)^2} = \frac{16\pi m^2 \alpha^2}{\hbar^4 \kappa^2 (4k^2 + \kappa^2)}$$

(??? тоже нужно пересчитать интеграл!)
Кулоновский потенциал: $\kappa \to 0$:

$$f(\theta) = -\frac{m\alpha}{2\hbar^2 k^2 \sin^2\frac{\theta}{2}} \qquad \Rightarrow \qquad \sigma = \frac{\pi m^2 \alpha^2}{2\hbar^4 k^4} \int\limits_0^\pi \frac{\sin\theta d\theta}{\sin^4\frac{\theta}{2}} \to \infty$$

physicspages.com 1D delta function in Born approximation

The delta function well.

$$V = -\alpha\delta(x)$$

Reminder: one-dimensional Born approximation is

$$R = \left(\frac{m}{\hbar^2 k}\right)^2 \left| \int\limits_{-\infty}^\infty e^{2ikx} V(x) dx \right|^2$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

Solution

$$\begin{aligned} R &= \left(\frac{m}{\hbar^2 k}\right)^2 \left|-\alpha e^{2ik\times 0}\right|^2 \\ &= \frac{m\alpha^2}{2\hbar^2 E} \\ T &= 1 - R = 1 - \frac{m\alpha^2}{2\hbar^2 E} \end{aligned}$$

The exact values are

$$\begin{aligned} R &= \frac{1}{1 + 2\hbar^2 E/m\alpha^2} \\ T &= \frac{1}{1 + m\alpha^2/2\hbar^2 E} \end{aligned}$$

For a weak potential, α is small, so $2\hbar^2 E/m\alpha^2 \gg 1$ so we can approximate the exact formulas by

$$\begin{aligned} R &\approx \frac{1}{2\hbar^2 E/m\alpha^2} = \frac{m\alpha^2}{2\hbar^2 E} \\ T &\approx 1 - \frac{m\alpha^2}{2\hbar^2 E} \end{aligned}$$

in agreement with the Born approximation.

physicspages.com 1D well in Born approximation

Here

$$V = \begin{cases} -V_0 & -a < x < a \\ 0 & \text{otherwise} \end{cases}$$

Reminder: one-dimensional Born approximation is

$$\begin{aligned} R &= \left(\frac{m}{\hbar^2 k}\right)^2 \left| \int_{-\infty}^{\infty} e^{2ikx} V(x) dx \right|^2 \\ k &= \frac{\sqrt{2mE}}{\hbar} \end{aligned}$$

Solution

$$\int_{-\infty}^{\infty} e^{2ikx} V(x) dx = -V_0 \int_{-a}^{a} e^{2ikx} dx = -V_0 \frac{e^{2ika} - e^{-2ika}}{2ik} = -\frac{V_0}{k} \sin(2ka)$$

$$\begin{aligned} R &= \left(\frac{m}{\hbar^2 k}\right)^2 \left| -\frac{V_0}{k} \sin(2ka) \right|^2 = \frac{V_0^2}{4E^2} \sin^2\left(\frac{2a\sqrt{2mE}}{\hbar}\right) \\ T &= 1 - \frac{V_0^2}{4E^2} \sin^2\left(\frac{2a\sqrt{2mE}}{\hbar}\right) \end{aligned}$$

The exact formula is

$$T^{-1} = 1 + \frac{V_0^2}{4E\,(E + V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m\,(E + V_0)}\right)$$

For a weak potential (or, equivalently, a high incident energy), $E \gg V_0$ and we get

$$\begin{aligned} T^{-1} &\approx 1 + \frac{V_0^2}{4E^2} \sin^2\left(\frac{2a\sqrt{2mE}}{\hbar}\right) \\ T &\approx 1 - \frac{V_0^2}{4E^2} \sin^2\left(\frac{2a\sqrt{2mE}}{\hbar}\right) \end{aligned}$$

so again, the Born approximation gives a good result.

GKKG.13.2 Cross-sections in the Born approximation

Prove that the total scattering cross-section (in the Born approximation) of a high energy particle in a potential, $U(r)$ with $kR \gg 1$ is described by the expression

$$\sigma(E)|_{E\to\infty} \approx \frac{m}{2\hbar^2 E} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} U(\rho, z)dz\right]^2 d^2\rho \tag{1}$$

The momentum of the particle before scattering is along the z-axis; $\boldsymbol{\rho}$ is a twodimensional radius-vector lying in the plane perpendicular to the z-axis.

Apply this result to the potential $U(r) = U_0 \exp\left\{-r^2/R^2\right\}$ and to a rectangular potential well (barrier) of strength, U_0, and radius, R. Compare to Problem 13.1.

Prove also that, in this case, the transport scattering cross-section has an asymptotic behavior given by

$$\sigma_{tr} = \int (1-\cos\theta)d\sigma\Big|_{E\to\infty} \approx \frac{1}{8E^2}\iint \left[\int_{-\infty}^{\infty} \frac{\rho}{r}\frac{\partial U(r)}{\partial r}dz\right]^2 d^2\rho \tag{2}$$

State conditions of applicability for these results.

Solution

From Eq. (XIII.6), the scattering amplitude is related to the Fourier transform of the potential, $\tilde{U}(\mathbf{q})$, with

$$f_B(\mathbf{q}) = -\frac{m}{2\pi\hbar^2}\tilde{U}(\mathbf{q}), \quad \tilde{U}(\mathbf{q}) = \int e^{-i\mathbf{q}\cdot\mathbf{r}}U(r)dV$$

From this, it follows that $f_B(q)$ is essentially different from zero only if $qR \lesssim 1$ (where R is the range of the potential); for $qR \gg 1$, this the integral is small due to the fast oscillating integrand. Since $q^2 = 2k^2(1-\cos\theta)$, the two conditions, $kR \gg 1$ and $qR \leq 1$, lead to the known conclusions that the scattering of fast particles occurs primarily into small angles, $\theta \sim 1/kR \ll 1$. From this, it follows that $q \approx k\theta \sim R^{-1}$.

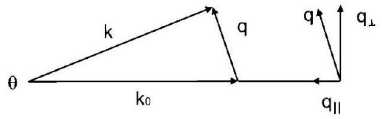


Fig. 13.1

For what follows, we decompose $\mathbf{q}$ into two perpendicular components, $\mathbf{q} = \mathbf{q}_{\|} + \mathbf{q}_{\perp}$, where $\mathbf{q}_{\|}$is directed along the incident momentum, $\hbar\mathbf{k}_0$ (see Fig. 13.1). For $\theta \ll 1$, we have

$$q_{\|} = k(1-\cos\theta) \approx \frac{1}{2}k\theta^2, \quad q_{\perp} = k\sin\theta \approx k\theta$$

so that $q_{\perp} \gg q_{\|}$. It is safe to consider $\mathbf{q} \approx \mathbf{q}_{\perp}$, so that

$$\tilde{U}(\mathbf{q}) \approx \tilde{U}\left(\mathbf{q}_{\perp}\right) = \iiint e^{-i\mathbf{q}_{\perp}\cdot\boldsymbol{\rho}}U(\boldsymbol{\rho}, z)dzd^2\rho \tag{3}$$

To find the scattering cross-section we will carry out the q-integration only in a small region of the 4π-sphere around the z-axis. This region can be considered as approximately flat, so that $k^2 d\Omega \approx dS = dq_{\perp x}dq_{\perp y} = d^2q_{\perp}$. Therefore,

$$\sigma(E) = \int |f_B|^2 d\Omega \approx \frac{m^2}{4\pi^2\hbar^4k^2}\iint \left|\tilde{U}\left(\mathbf{q}_{\perp}\right)\right|^2 d^2q_{\perp}$$

Using expression (3), we have

$$\sigma(E) = \frac{m}{8\pi^2\hbar^2E}\iint \left[\iiint e^{-i\mathbf{q}_{\perp}\cdot\boldsymbol{\rho}}U(\boldsymbol{\rho}, z)dzd^2\rho\right]\left[\iiint e^{i\mathbf{q}_{\perp}\cdot\boldsymbol{\rho}'}U\left(\boldsymbol{\rho}', z'\right)dz'd^2\rho'\right]d^2q_{\perp}$$

After performing the $\mathbf{q}_{\perp}$-integration using

$$\iint \exp\left\{-i\mathbf{q}_{\perp}\cdot\left(\boldsymbol{\rho}-\boldsymbol{\rho}'\right)\right\}d^2q_{\perp} = (2\pi)^2\delta\left(\boldsymbol{\rho}-\boldsymbol{\rho}'\right) \tag{4}$$

and the resulting δ-function integration over ρ', we are immediately led to the following asymptote of the scattering cross-section:

$$\sigma(E)_{E\to\infty} = \frac{m}{2\hbar^2 E}\iint\left[\int\limits_{-\infty}^{\infty} U(\boldsymbol{\rho}, z)dz\right]^2 d^2\rho$$

For the potential $U(r) = U_0 \exp\left\{-r^2/R^2\right\}$ and the rectangular well (barrier), using this expression, we obtain

$$\sigma(E) = \frac{\pi^2 m U_0^2 R^4}{4\hbar^2 E} \quad \text{and} \quad \sigma(E) = \frac{\pi m U_0^2 R^4}{\hbar^2 E}$$

respectively (see Problem 13.1 e, f, they are the same).

2) Finding energy-dependence of the transport cross section for $E \to \infty$

$$\sigma_{tr}(E) = \int(1-\cos\theta)d\sigma\Big|_{E\to\infty} \approx \frac{m}{8\pi^2\hbar^4 k^4}\iint q_\perp^2\left|\tilde{U}\left(q_\perp\right)\right|^2 d^2 q_\perp \tag{5}$$

Now, instead of Eq. (4), we use the integral

$$\iint q^2 e^{-iq\cdot\rho}d^2q = -(2\pi)^2\Delta_\perp\delta(\boldsymbol{\rho})$$

Following some transformations in Eq. (5) for the case of a spherically-symmetric potential, we obtain the desired asymptotic form:

$$\sigma_{tr}(E)|_{E\to\infty} \approx \frac{1}{8E^2}\iint\left[\int\limits_{-\infty}^{\infty}\frac{\rho}{r}\frac{\partial U}{\partial r}dz\right]^2 d^2\rho$$

Note that this expression does not contain Planck's constant, and coincides with σ_{tr} for fast particles ($E \gg U$) in classical mechanics, defined as

$$\sigma_{tr,\ \text{class}}\ (E) = \int\limits_0^\infty[1-\cos\theta(\rho)]\cdot 2\pi\rho d\rho \approx \pi\int\limits_0^\infty\theta^2(\rho)\rho d\rho$$

We have used an equation for small-angle scattering from classical mechanics.
The agreement of the result of Born approximation with the classical result at first sight might appear strange. However, it becomes less surprising if we recall that the same result follows from the quasi-classical eikonal approximation (XIII.18) too; Compare to the Rutherford equation.

In conclusion, we note that expression in Eq. (2) assumes that the differential scattering cross-section at large momenta falls faster than $\propto q^{-2}$, so that the upper limit of the q^2-integration could be set to infinity.

GKKG.13.3 Scattering of exchange potential

Using Born approximation, obtain an expression for the scattering amplitude of a particle in an exchange potential; that is, $\hat{U}_{exc}\psi(\mathbf{r}) \equiv U(r)\psi(-\mathbf{r})$.

Find how the scattering amplitude in this case is related to the scattering amplitude of the particle in a regular garden-variety potential, $U(r)$. Obtain the angular distribution of fast particles.

Solution

Substituting $U\psi^+_{\mathbf{k}_0}$ in Eqs. (XIII.4, 5) by $\hat{U}_{ex}\psi^+_{\mathbf{k}_0}, \psi^+_{\mathbf{k}_0}(\mathbf{r})$ by $e^{i\mathbf{k}_0\cdot\mathbf{r}}$, and taking into account the exchange nature of $\hat{U}_{ex}$, we find

$$f^B_{ex}\left(\mathbf{k}_0, \mathbf{k}\right) = f^B_{ex}(\boldsymbol{\Delta}) = -\frac{m}{2\pi\hbar^2}\int e^{-i\boldsymbol{\Delta}\cdot\mathbf{r}}U(r)dV \tag{1}$$

where $\boldsymbol{\Delta} = \mathbf{k} + \mathbf{k}_0$ and $\Delta^2 = 2k^2(1+\cos\theta)$. Thus,

$$f^B_{ex}(E,\theta) = f^B(E, \pi-\theta)$$

where $f^B(E,\theta)$ is the amplitude of scattering in a regular spherically-symmetric potential, $U(r)$. From this relation, it is clear that for fast particles ($kR \gg 1$), the scattering from the exchange potential occurs primarily "backwards," with the relevant angles, $\pi - \theta \lesssim (kR)^{-1}$. For more on scattering from an exchange potential, see Problem 13.56.

GKKG.13.4;Б-2.12.13 Scattering of electrons and a hydrogen atom

Find the differential and total cross-section of elastic scattering of fast electrons by a hydrogen atom in its ground state. Neglect a polarization of the atom. See also Problem 13.77.

Solution

The scattering potential is of the form:

$$U(r) = -e^2\left(\frac{1}{r} + \frac{1}{a_B}\right)e^{-2r/a_B}$$

(see Problem 4.6). According to Eq. (XIII.8),

```
Integrate[(1/r+1/a) Exp[-2r/a] r Sin[q r],{r,0,Infinity},
Assumptions->{q>0,a>0,Im[a q]==0}]
```

$$f^B(q) = \frac{2\left(8 + q^2a_B^2\right)}{\left(4 + q^2a_B^2\right)^2}a_B \tag{1}$$

The total scattering cross-section $\left(d\Omega = \pi k^{-2}dq^2\right)$:

$$\sigma = \frac{\pi}{k^2}\int\limits_0^{4k^2}\left(f^B\right)^2 dq^2 = \frac{4\pi}{k^2}\left[\frac{7}{12} - \frac{7 + 9k^2a_B^2 + 3k^4a_B^4}{12\left(1 + k^2a_B^2\right)^3}\right] \approx \frac{7\pi a_B^2}{3\left(ka_B\right)^2} \tag{2}$$

Here, we have taken into account the condition of applicability of the Born approximation (XIII.7), viz. $ka_B \gg 1$. (See also Problems 13.77 and 13.78)

Solution. Белоусова

Для описания упругого рассеяния быстрых электронов на атоме (не обязательно на атоме водорода) можно использовать борновское приближение, если скорость налетающего электрона велика по сравнению со скоростями атомных электронов. Поскольку масса атома гораздо больше, чем масса электрона, можно считать, что атом является неподвижным в течение всего процесса рассеяния. Тогда в формуле борновского приближения

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\int e^{-i\mathbf{qr}}V(r)d^3x, \quad \mathbf{q} = \mathbf{k}' - \mathbf{k},$$

как и обычно, $\hbar\mathbf{k}$ и $\hbar\mathbf{k}'$ - импульсы электрона до и после рассеяния, m - масса электрона.

С точки зрения воздействия на электрон, атом представляет собой систему зарядов. Это распределение зарядов создает электрический потенциал, на котором и рассеивается заряженная частица. Потенциал атома создается зарядом ядра и зарядом электронов, распределенным по объему атома, т. е.

$$V(r) = -\frac{Ze^2}{r} + e^2\int\frac{\rho\left(r'\right)}{|\mathbf{r} - \mathbf{r}'|}d^3x',$$

где $-e\rho(r)$ - плотность заряда электронов в атоме. Подставляя $V(r)$ в выражение (1) и учитывая значения интегралов

$$\int\frac{1}{r}e^{-i\mathbf{qr}}d^3x = \frac{4\pi}{q^2}, \int\frac{e^{-iq\boldsymbol{q}}}{|\mathbf{r} - \mathbf{r}'|}d^3x = \frac{4\pi}{q^2}e^{-i\mathbf{q}r'},$$

получаем

$$f(\theta) = \frac{2me^2}{\hbar^2q^2}[Z - F(q)], \quad \text{где} \quad F(q) = \int\rho(r)e^{-iqr}d^3x.$$

Выражение (2) определяет так называемый атомный формфактор. Он зависит от распределения плотности электронов в атоме и от величины q - передаваемого при рассеянии импульса. Если плотность электронов обладает центральной симметрией, то формулу (2) можно упростить:

$$F(q) = \frac{4\pi}{q}\int\limits_0^\infty \sin qr\rho(r)rdr.$$

Для атома водорода ($Z = 1$), находящегося в основном состоянии, электронная плотность $\rho(r)$ определяется очевидным образом:

$$\rho(r) = |\psi_{100}(r)|^2 = \frac{1}{\pi a^2} e^{-2r/a},$$

фактор

$$F(q) = \left[1 + \frac{(qa)^2}{4}\right]^{-2}.$$

Определяем далее дифференциальное сечение рассеяния

$$d\sigma = 4a^2 \frac{\left((qa)^2 + 8\right)^2}{\left((qa)^2 + 4\right)^4} d\Omega.$$

Для вычисления полного сечения заметим, что $d\Omega = 2\pi \sin\theta d\theta = \left(2\pi/k^2\right) qdq$, поскольку $q = 2k \sin\theta/2$. В итоге имеем

$$\sigma = \frac{\pi a^2}{3} \frac{7(ka)^4 + 72(ka)^2 + 192}{\left((ka)^2 + 4\right)^3}\bigg|_{ka \gg 1} \simeq \frac{7\pi}{3k^2}.$$

Критерий применимости борновского приближения (если положить $V_0 \sim e^2/a$) дает условие $ka \gg 1$, поэтому данное приближение применимо лишь для достаточно больших энергий налетающих электронов.

GKKG.13.5 Scattering of electrons and a helium

Find the differential and total cross-section of elastic scattering of fast electrons by a helium atom in its ground state. Neglect a polarization of the atom. Choose the atomic wavefunction using the variational calculation performed in Problem 11.6.

Solution

In the approximation considered in Problem 11.6, we found that the mean electronic density in the ground state of a helium atom is $n = \frac{2}{\pi a^3} e^{-2r/a}$, where $a = a_B/Z_{\text{eff}} = 16a_B/27$. From this, we calculate the form-factor:

$$F(\mathbf{q}) = \int n(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} dV = \frac{2}{\pi a^3} \int e^{-2r/a - i\mathbf{q}\cdot\mathbf{r}} dV = \frac{32}{\left(4 + q^2a^2\right)^2}$$

Here first we evaluate $\int ..d\theta$ and from exponent sine pops up. Later we can integrate by parts of just use:

```
Integrate[Exp[-2r/a] r Sin[q r],{r,0,Infinity},Assumptions->{q>0,a>0,Im[a q]==0}]
```

Using the known equation, (?? maybe it is written in theory of helium in GKKG???)

$$\frac{d\sigma}{d\Omega} = \frac{4[Z - F(q)]^2}{q^4 a_B^2}$$

we find the differential and total cross-section of elastic scattering from the helium atom:

```
Integrate[4 (2 - 32/(4 + qq a^2)^2)^2/(qq^2 a^2), {qq, 0, 4 k},
 Assumptions -> {k > 0, a > 0, Im[a q k] == 0}]
```

(don't even want to think about evaluation of this integral, but maybe it can be done using complex analysis)

$$\sigma = \frac{\pi}{k^2} \int_0^{4k^2} \frac{d\sigma}{d\Omega} dq^2 = \frac{4\pi a^2}{k^2 a_B^2} \frac{7k^6a^6 + 18k^4a^4 + 12k^2a^2}{3\left(1 + k^2a^2\right)^3} \overset{ka_B \gg 1}{\approx} \frac{28\pi a^2}{3\left(ka_B\right)^2}$$

We have $ka_B \gg 1$, and the total cross-section differs from the cross-section for scattering from the hydrogen atom by the factor $4(16/27)^2 \approx 1.40$.

GKKG.13.6 Z-dependance of the cross-section

Find the Z-dependance of the cross-section for the elastic scattering of fast electrons by a neutral atom with $Z \gg 1$; use the Thomas-Fermi model for the interaction potential.

Solution

(!!! I'll add it to the 1st part!)
Under the Thomas-Fermi approximation, the interaction potential between the scattered electrons and the neutral atom (ignoring an atom polarization) is

$$U(r) = -\varphi(r) = -\frac{Z}{r}\chi\left(\frac{rZ^{1/3}}{b}\right)$$

where $\chi(x)$ is the universal function in the Thomas-Fermi model (see Eq. (XI.3). We use the atomic system of units $e = \hbar = m_e = 1$.) The scattering amplitude in the Born approximation is

$$f^B(Z,q) = -2\int\limits_0^\infty U(r)\frac{\sin qr}{q}rdr = Z^{1/3}\Phi\left(\frac{q}{Z^{1/3}}\right) \tag{1}$$

where $\Phi(x)$ is a new universal function (the same for all atoms):

$$\Phi(x) = \frac{2}{x}\int\limits_0^\infty \chi\left(\frac{y}{b}\right)\sin(xy)dy \tag{2}$$

As $x \to \infty$, only a small region of y in the vicinity of the lower limit contributes to the integral (2). Taking into account that $\chi(0) = 1$ and $\int\limits_0^\infty \sin y dy = 1$ (the usual procedure is to introduce a "cutoff" factor $e^{-\alpha y}$ with $\alpha > 0$ in the integrand, and in the final result take the limit $\alpha \to 0$), we find $\Phi(x) \approx 2/x^2$, as $x \to \infty$.
(??? need to practice with it more!!!)
Hence, from Eq. (1), we have

$$f^B_{q\gg Z^{1/3}} \approx 2Z/q^2.$$

It is not unexpected that this corresponds to the amplitude of Rutherford electron scattering in atomic nuclei, since for a large momentum transfer, the screening by atomic electrons can be ignored. As $x \to 0$, the function $\Phi(x)$ takes a finite value.
Eqs. (1) and (2) give the differential cross-section of elastic scattering; the total scattering cross-section is given by

$$\sigma = \frac{\pi}{k^2}\int\limits_0^{4k^2}\left[f^B(q)\right]^2 dq^2 \approx \frac{\pi Z^{2/3}}{k^2}\int\limits_0^\infty \Phi^2\left(\frac{q}{Z^{1/3}}\right)dq^2 = \pi C\frac{Z^{4/3}}{k^2}$$

where $C = 7.14$.
(???? пока нет идей, как последний интеграл взят????)

GKKG.13.7 Collision of identical potentials and diatomic molecules

Using the Born approximation, find the amplitudes for scattering from two identical potential centers that are at some distance, a, from each other (viz., of the form $U(\mathbf{r}) = U_0(r) + U_0(|\mathbf{r} - \mathbf{a}|)$). Express your answer in terms of the scattering amplitude, $f_0^B(q)$, for scattering from $U_0(r)$ alone.
From this expression, determine a relation between the differential cross-sections for scattering of fast electrons from monoatomic and homonuclear diatomic molecules. Note that this quantity should be averaged over the molecular axis orientations, considering all of them to appear with equal probability.
Find a relation between the total scattering cross-sections from one and two centers for the following limiting cases:
a) $ka \ll 1$ (here the quantity $kR - R$ being the range of potential $U_0(r)$ - could be arbitrary);
b) $kR \sim 1$ and $a \gg R$ (i.e., the distance between the centers is much larger than the range of $U_0(r)$).

Solution

(про это отдельно подумаю, в 1ю часть добавлю, там есть раздел про рассеяние на решетке)
The scattering amplitude for two identical force centers separated by a distance, $\mathbf{a}$, is given by

$$f^B_{2c}(\mathbf{q}) = -\frac{m}{2\pi\hbar^2}\int e^{-i\mathbf{q}\cdot\mathbf{r}}\left[U_0(r) + U_0(|\mathbf{r} - \mathbf{a}|)\right]dV = f_0^B(q)\left[1 + e^{-i\mathbf{q}\cdot\mathbf{a}}\right] \tag{1}$$

from which the differential scattering cross-section follows:

$$\frac{d\sigma_{2c}}{d\Omega} = 2(1 + \cos \mathbf{q} \cdot \mathbf{a}) \left[f_0^B(q)\right]^2 \tag{2}$$

Although the form of the potential implies two identical force centers, the expressions in (1) and (2) are also applicable to a diatomic molecule. This is because only the valence electrons participate in the molecular formation, leaving behind two inner cores (nuclei screened by inner electrons) that are essentially the same as those of two isolated atoms. However, Eq. (2) must be averaged over all a. Neglecting nuclear vibrations (see Problem 11.25), it is sufficient to average only over the directions of a. For an isotropic distribution, this means that we perform the averaging using a direction-element $dw = d\Omega_{\rm n}/4\pi$ ($d\Omega_{\rm n}$ is an infinitesimal element of the solid angle that includes the direction of the vector $\mathbf{a} = a\mathbf{n}$). We obtain (choosing the z-axis along $\mathbf{q}$):

$$\overline{\cos \mathbf{a} \cdot \mathbf{q}} = \frac{1}{4\pi} \int \cos \mathbf{a} \cdot \mathbf{q} d\Omega_n = \frac{\sin qa}{qa}$$

Thus,

$$\frac{d\sigma_{mol}}{d\Omega} = 2\left(1 + \frac{\sin qa}{qa}\right) \frac{d\sigma_{at}}{d\Omega}$$

As can be seen, the relation between the atomic and the molecular scattering crosssections changes with the distance between the nuclei, a. (Similar relations can be found for multiatomic molecules, even heterogeneous ones. They form the basis of the diffraction methods used for examining molecular structures.)

Let us discuss the relation between the total scattering cross-sections. For $ka \ll 1$ and $qa \ll 1$, $f_{2c}^B \approx 2f_0^B$, the scattering cross-section on two centers is four times larger than on a single center. In the cases $kR \leq 1$ and $a \gg R$, we have $ka \gg 1$, and hence the quantity qa changes essentially, even for a small change of the scattering angle. So, in the integration (2) over the angles, the term with the fast oscillating factor, $\cos(\mathbf{q} \cdot \mathbf{a})$, is much smaller than the first term, so that in this case the cross-section of scattering on two centers is twice as large as on one center.

GKKG.13.8 Formula for N identical centers

Generalize the result of the previous problem for the case of a system with arbitrary number N of identical centers, located at the points $\mathbf{a}_n, n = 1, 2, ..., N$.

Discuss properties of the angular distribution of the scattered particles for an ordered array of a large number ($N \gg 1$) of centers along a straight line with the same distance, b, between closest neighbors.

Solution

In the Born approximation, the scattering amplitude is described by the expression (compare to the previous problem):

$$f_N^B(\mathbf{q}) = f_0^B(q) G_N(\mathbf{q}), \quad G_N(\mathbf{q}) = \sum_n e^{-i\mathbf{q}\cdot\mathbf{a}_n} \tag{1}$$

Let us emphasize that the factor $G_N(\mathbf{q})$ depends only on the mutual position of the centers and on the vector $\mathbf{q}$ (but not on the form of interaction between the particle and a single center).

In the case of an array of potential centers ordered along a line with the unit vector $\mathbf{j}$ ($\mathbf{a}_n = b(n-1)\mathbf{j}$), we have

$$G_N = \sum_{n=1}^{N} \exp\{-ib(n-1)\mathbf{q} \cdot \mathbf{j}\} = \frac{1 - \exp\{-ibN\mathbf{q} \cdot \mathbf{j}\}}{1 - \exp\{-ib\mathbf{q} \cdot \mathbf{j}\}}$$

$$|G_N(\mathbf{q})|^2 = \left[\frac{\sin(bN\mathbf{q} \cdot \mathbf{j}/2)}{\sin(b\mathbf{q} \cdot \mathbf{j}/2)}\right]^2 \tag{2}$$

In the case of $N \gg 1$, the quantity $|G_N(\mathbf{q})|^2$ is especially large for specific values, $\mathbf{q} = \mathbf{q}_s$ with [316] $b\mathbf{q}_s \cdot \mathbf{j} = 2\pi s$, where $s = 0, \pm 1, \pm 2, ...$ So, the particles are scattered mostly into particular directions, for which

$$\cos \beta_s \approx \frac{\mathbf{k}_0 \cdot \mathbf{j}}{k_0} + \frac{2\pi s}{bk_0}$$

[316] Restriction on $|s|_{\max}$ is determined by the momentum of scattered particles. In the case of $k < \pi/b$, only the value $s = 0$ is possible. In this case, $q = 0$, so that coherent scattering is absent.

where β_s is the angle between the vectors $\mathbf{k}$ and $\mathbf{j}$ (note that $\mathbf{qj} = \mathbf{kj} - \mathbf{k}_0\mathbf{j}$). At maximum, $|G_N|^2 = N^2$. The maxima are sharp; their width is $\Delta\beta_s \propto 1/\sqrt{N}$. The scattering cross-section into such interval of angles is $\propto N$. For other scattering angles, $|G_N|^2 \sim 1$

These results could be obtained by taking advantage of the large- N limit in the expression for $|G_N|^2$. Using the relation

$$\lim_{N\to\infty} \frac{\sin^2 \alpha N}{\pi \alpha^2 N} = \delta(\alpha)$$

and expanding $\sin(b\mathbf{q}\cdot\mathbf{j}/2)$ in expression (2) in the vicinity of $\mathbf{q}_s$, we find

$$|G_N(\mathbf{q})|^2 \approx \frac{2\pi N}{b} \sum_{s=-\infty}^{\infty} \delta\left(\mathbf{k}\cdot\mathbf{j} - \mathbf{k}_0\cdot\mathbf{j} - \frac{2\pi s}{b}\right) \tag{3}$$

Such method allows for an easy generalization to the case of a "crystalline" arrangement of the scattering centers. In particular, for a system of centers with $\mathbf{a}_{\{n\}} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3, n_a = 0, 1, ..., N_a - 1$, we have [317] ([317] Here we have used the relation: $\prod_{a=1}^{3} \delta(\mathbf{q}\cdot\mathbf{b}_a - 2\pi s_a) = \frac{1}{b_1 b_2 b_3}\delta(\mathbf{q} - 2\pi\boldsymbol{\tau})$)

$$|G_N(\mathbf{q})|^2 = \left|\sum_{\{n\}} \exp\left\{-i\mathbf{q}\cdot\mathbf{a}_{\{n\}}\right\}\right|^2 = \frac{(2\pi)^3 N}{b_1 b_2 b_3} \sum_{\tau} \delta\left(\mathbf{k} - \mathbf{k}_0 - 2\pi\boldsymbol{\tau}\right) \tag{4}$$

where $N = N_1 \cdot N_2 \cdot N_3$ is the total number of scattering centers,

$$\boldsymbol{\tau} = s_1\mathbf{a}_1 + s_2\mathbf{a}_2 + s_3\mathbf{a}_3, \quad s_a = 0, \pm 1, ...,$$

$$\mathbf{a}_1 = \frac{1}{\Delta}\left[\mathbf{b}_2 \times \mathbf{b}_3\right], \quad \mathbf{a}_2 = \frac{1}{\Delta}\left[\mathbf{b}_3 \times \mathbf{b}_1\right], \quad \mathbf{a}_3 = \frac{1}{\Delta}\left[\mathbf{b}_1 \times \mathbf{b}_2\right], \quad \Delta = (\mathbf{b}_1 \cdot [\mathbf{b}_2 \times \mathbf{b}_3])$$

(where $\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = \mathbf{a}_3 \cdot \mathbf{b}_3 = 1$).
The δ-function terms in Eq. (4) determine the directions, $\mathbf{k} = \mathbf{k}_0 + 2\pi\boldsymbol{\tau}$, of particle elastic scattering in crystals (Bragg's law).

GKKG.13.9 Collision of extended particles

In the Born approximation, find the scattering amplitude for the collision of two extended (non-point-like) particles, interacting with each other via electrostatic forces. The particles are considered to be extended, which means they are characterized by some charge distribution, $\rho_{1,2}(r)$, that is assumed to be spherically symmetric with respect to the center of mass of the corresponding particle and does not change in the collision process. Express the scattering amplitude in terms of the charge distributions, $\rho_{1,2}(r)$, and the form-factors $F_{1,2}(q)$.

Solution

(тоже строчку в 1ю добавлю про такой случай)
The interaction potential is

$$U(r) = \iint \frac{\rho_1(r_1')\,\rho_2(r_2')}{|\mathbf{r} + \mathbf{r}_1' - \mathbf{r}_2'|} dV_1' dV_2'$$

where $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, and $\mathbf{r}_{1,2}$ are the radius vectors of the centers of mass of the colliding particles. Taking into account the relation

$$\int \frac{e^{-i\mathbf{q}\cdot\mathbf{r}} dV}{|\mathbf{r} + \mathbf{r}_1' - \mathbf{r}_2'|} = \frac{4\pi}{q^2} e^{i\mathbf{q}\cdot(\mathbf{r}_1' - \mathbf{r}_2')}$$

and according to Eq. (XIII.6), we obtain

$$f^B(q) = -\frac{2m}{\hbar^2 q^2} F_1(q) F_2(q)$$

(where m is the reduced mass of the particles). Here,

$$F_{1,2}(q) = \int e^{-i\mathbf{q}\cdot\mathbf{r}} \rho_{1,2}(r) dV$$

are the form-factors of the corresponding charge distributions. Note that $F_{1,2}(0) = e_{1,2}$ are particle charges. Some properties of the form-factors are considered in Problems 13.80 and 13.84.

By the way, the fact that charge distribution is not point-like denotes the composite character of colliding particles (compare, for example, to Problem 13.4). Since, though, the change of their inner states in a collision process is to be neglected, then the problem is reduced to a common problem of two-body scattering. In connection with this problem, see also Problem 13.80.

17.3.8 Problems about scattering in Born approximation 2

GKKG.13.10 Formula for n-th order of general formula

Obtain an expression for the scattering amplitude in the n-th order of perturbation theory for a potential $U(r)$.

Hint: First, using Eqs. (XIII.5) and (XIII.4), obtain an integral equation for the scattering amplitude (the Lippmann-Schwinger equation).

Solution

Substituting expression (XIII.4) into Eq. (XIII.5), and using the momentum representation for the free-particle Green function,

$$\frac{e^{ik_0|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{2\pi^2}\int \frac{e^{i\boldsymbol{\kappa}\cdot(\mathbf{r}-\mathbf{r}')}}{\kappa^2-k_0^2-i\varepsilon}d^3\kappa$$

($\varepsilon > 0, \varepsilon \to 0$), we obtain the Lippmann-Schwinger equation:

$$f(\mathbf{k},\mathbf{k}_0) = -\frac{m}{2\pi\hbar^2}\left[\tilde{U}(\mathbf{k}-\mathbf{k}_0) + \int \frac{\tilde{U}(\mathbf{k}-\boldsymbol{\kappa})f(\boldsymbol{\kappa},\mathbf{k}_0)}{2\pi^2(\kappa^2-k_0^2-i\varepsilon)}d^3\kappa\right] \tag{1}$$

Let us emphasize that for physical real elastic scattering, $k^2 = k_0^2 = 2mE/\hbar^2$. On the other hand, Eq. (1) connects the scattering amplitudes for values $k^2 \neq k_0^2$ (outside the physical sheet or so-called energy surface; see also Eq. (XIII.5)).

Using Eq. (1), we find a recurrence relation for the terms in the expansion, $f(\mathbf{k},\mathbf{k}_0) = \sum\limits_n f^{(n)}$, of the scattering amplitude in powers of interaction, and then obtain an explicit expression for them ($\mathbf{q} = \mathbf{k}-\mathbf{k}_0$):

$$f^{(1)}(\mathbf{k},\mathbf{k}_0) = f^B(\mathbf{q}) = -\frac{m}{2\pi\hbar^2}\tilde{U}(\mathbf{q}), \quad \tilde{U}(\mathbf{q}) = \int e^{-i\mathbf{q}\cdot\mathbf{r}}U(\mathbf{r})dV$$

$$f^{(n)}(\mathbf{k},\mathbf{k}_0) = \left(-\frac{m}{2\pi\hbar^2}\right)^n \int ... \int \tilde{U}(\mathbf{k}-\boldsymbol{\kappa}_{n-1})\frac{\tilde{U}(\boldsymbol{\kappa}_{n-1}-\boldsymbol{\kappa}_{n-2})\,d^3\kappa_{n-1}}{2\pi^2(\kappa_{n-1}^2-k_0^2-i\varepsilon)} ... \frac{\tilde{U}(\boldsymbol{\kappa}_1-\mathbf{k}_0)\,d^3\kappa_1}{2\pi^2(\kappa_1^2-k_0^2-i\varepsilon)} \tag{2}$$

GKKG.13.11 Connection of Born approximation and optical theorem

In the Born approximation, the forward scattering amplitude (angle $\theta = 0$) is a real quantity and so does not satisfy the optical theorem (XIII.11). Why does this fact not contradict the successful description of differential and total scattering cross-section in the framework of the Born approximation, whenever it applies?

Write an expression for the scattering amplitude in second-order perturbation theory. Find $\operatorname{Im} f^{(2)}(E,\theta=0)$ and explain the result obtained.

Solution

The Born approximation is the first linear term in the expansion of the scattering amplitude in power of the interaction (more specifically, of parameters given in Eq. (XIII.7)). On the other hand, an expansion of the scattering cross-section begins from the term quadratic in interaction, since $\sigma \propto |f|^2$. So, in the relation $4\pi \operatorname{Im} f(E,0) = k\sigma(E)$, the left-hand side must have a second-order interaction term, as the right-hand side does. It follows that necessarily $\operatorname{Im} f^B(\theta=0) = 0$.

In the 2nd order of perturbation theory, the scattering amplitude is described by expression (2) of the previous problem. In particular, for forward scattering ($\theta = 0$, $\mathbf{k} = \mathbf{k}_0$), it gives

$$f^{(2)}(\mathbf{k}_0,\mathbf{k}_0) = \frac{m^2}{8\pi^4\hbar^4}\int \frac{\left|\tilde{U}(\boldsymbol{\kappa}-\mathbf{k}_0)\right|^2}{\kappa^2-k_0^2-i\varepsilon}d^3\kappa \tag{1}$$

We used the fact that $\tilde{U}(\mathbf{q}) = \tilde{U}^*(-\mathbf{q})$. It follows that

$$\operatorname{Im} f^{(2)}(\mathbf{k}_0,\mathbf{k}_0) = \frac{m^2}{8\pi^4\hbar^4}\int \frac{\varepsilon}{(\kappa^2-k_0^2)^2+\varepsilon^2}\left|\tilde{U}(\boldsymbol{\kappa}-\mathbf{k}_0)\right|^2 d^3\kappa \tag{2}$$

If we note that [319] $\varepsilon/\pi\left(x^2+\varepsilon^2\right)=\delta(x)$ (for infinitesimal $\varepsilon>0$), and write $\boldsymbol{\kappa}=\kappa\mathbf{n}$, $d^3\kappa=\frac{1}{2}\kappa d\kappa^2 d\Omega_{\mathrm{n}}$, we transform expression (2) to the form

$$\operatorname{Im} f^{(2)}\left(\mathbf{k}_0,\mathbf{k}_0\right)=\frac{m^2}{16\pi^3\hbar^4}\iint\left|\tilde{U}\left(k\mathbf{n}-\mathbf{k}_0\right)\right|^2\kappa\delta\left(\kappa^2-k_0^2\right)d\kappa^2 d\Omega_{\mathbf{n}}=$$
$$\frac{m^2k_0}{16\pi^3\hbar^4}\int\left|\tilde{U}\left(k_0\mathbf{n}-\mathbf{k}_0\right)\right|^2 d\Omega_n\equiv\frac{k_0}{4\pi}\int\left|f^B\left(\mathbf{k}-\mathbf{k}_0\right)\right|^2 d\Omega_{\mathbf{n}}$$

i.e., $\operatorname{Im} f^{(2)}(E,\theta=0)=k\sigma_B(E)/4\pi$, which expresses the optical theorem in the 2nd order of perturbation theory.

physicspages.com 2nd order scattering on soft sphere

A soft sphere is defined by the potential

$$V(\mathbf{r})=\begin{cases}V_0 & r\le a\\ 0 & r>a\end{cases}$$

where $V_0>0$ is a constant. Griffiths works out the first order Born approximation for the scattering amplitude in his example 11.4, so calculate the second order term.

Reminding of the framework

The first order Born approximation in scattering theory is derived from the integral form of the Schrödinger equation

$$\psi(\mathbf{r})=\psi_0(\mathbf{r})+\int g\left(\mathbf{r}-\mathbf{r}_0\right)V\left(\mathbf{r}_0\right)\psi\left(\mathbf{r}_0\right)d^3\mathbf{r}_0$$

where

$$g\left(\mathbf{r}-\mathbf{r}_0\right)\equiv-\frac{m}{2\pi\hbar^2}\frac{e^{ik|\mathbf{r}-\mathbf{r}_0|}}{|\mathbf{r}-\mathbf{r}_0|}$$

is the Green's function and ψ_0 is a free particle wave function. The first order Born approximation assumes that the wave function isn't changed much by the scattering process, so we can approximate the integral equation by replacing the full wave function ψ in the integrand by the incident wave function:

$$\psi(\mathbf{r})=\psi_0(\mathbf{r})+\int g\left(\mathbf{r}-\mathbf{r}_0\right)V\left(\mathbf{r}_0\right)\psi_0\left(\mathbf{r}_0\right)d^3\mathbf{r}_0$$

We can generate a second order approximation by inserting 3 into the integral in 1 . When we do this, it's important to keep track of the position vectors that apply to each integration. We'll relabel $\mathbf{r}_0$ as $\mathbf{r}_1$ in 1, and then insert 3 into it:

$$\begin{aligned}\psi(\mathbf{r})=&\psi_0(\mathbf{r})+\int g\left(\mathbf{r}-\mathbf{r}_1\right)V\left(\mathbf{r}_1\right)\psi\left(\mathbf{r}_1\right)d^3\mathbf{r}_1\\ \approx&\psi_0(\mathbf{r})+\int g\left(\mathbf{r}-\mathbf{r}_1\right)V\left(\mathbf{r}_1\right)\psi_0\left(\mathbf{r}_1\right)d^3\mathbf{r}_1+\\ &\int g\left(\mathbf{r}-\mathbf{r}_1\right)V\left(\mathbf{r}_1\right)\int g\left(\mathbf{r}_1-\mathbf{r}_0\right)V\left(\mathbf{r}_0\right)\psi_0\left(\mathbf{r}_0\right)d^3\mathbf{r}_0 d^3\mathbf{r}_1\end{aligned}$$

The first two terms just repeat the first order Born approximation, so to calculate the second order approximation we need to work out the third term involving the double integral. Using 2 we have for this term (which we'll call I_2)

$$I_2=\left(\frac{m}{2\pi\hbar^2}\right)^2\iint\frac{e^{ik|\mathbf{r}-\mathbf{r}_1|}}{|\mathbf{r}-\mathbf{r}_1|}\left|\frac{e^{ik|\mathbf{r}_1-\mathbf{r}_0|}}{|\mathbf{r}_1-\mathbf{r}_0|}V\left(\mathbf{r}_1\right)V\left(\mathbf{r}_0\right)\psi_0\left(\mathbf{r}_0\right)d^3\mathbf{r}_0 d^3\mathbf{r}_1\right.$$

In the original derivation, we simplified things by taking $\mathbf{r}$ to point to the detector, which is assumed to be very far from the scattering region. This allows us to approximate the Green's function:

$$g\left(\mathbf{r}-\mathbf{r}_0\right)\approx-\frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}e^{-i\mathbf{k}\cdot\mathbf{r}_0}$$

This approximation is still valid for the first factor in the integrand in 6, but not for the second factor, since $\mathbf{r}_0$ and $\mathbf{r}_1$ are position vectors that both refer to locations within the scattering region (that is, where $V\neq0$). Therefore we can write

$$I_2\approx\left(\frac{m}{2\pi\hbar^2}\right)^2\frac{e^{ikr}}{r}\iint e^{-i\mathbf{k}\cdot\mathbf{r}_1}\frac{e^{ik|\mathbf{r}_1-\mathbf{r}_0|}}{|\mathbf{r}_1-\mathbf{r}_0|}V\left(\mathbf{r}_1\right)V\left(\mathbf{r}_0\right)\psi_0\left(\mathbf{r}_0\right)d^3\mathbf{r}_0 d^3\mathbf{r}_1$$

Solution

We'll also consider only the case of low energy scattering, which is defined by the condition $ka \ll 1$. We start by writing out 8 for this case.

$$I_2 \approx \left(\frac{m}{2\pi\hbar^2}\right)^2 \frac{e^{ikr}}{r} V_0^2 \iint e^{-i\mathbf{k}\cdot\mathbf{r}_1} \frac{e^{ik|\mathbf{r}_1-\mathbf{r}_0|}}{|\mathbf{r}_1-\mathbf{r}_0|} \psi_0(\mathbf{r}_0)\, d^3\mathbf{r}_0 d^3\mathbf{r}_1$$

To do the integral, we use an incident plane wave for ψ_0:

$$\psi_0(\mathbf{r}_0) = Ae^{i\mathbf{k}'\cdot\mathbf{r}_0}$$
$$\mathbf{k}' \equiv k\hat{\mathbf{z}}$$

If we do the $\mathbf{r}_0$ integration first, we can take the polar axis to be along $\mathbf{r}_1$. Then

$$|\mathbf{r}_1-\mathbf{r}_0| = \sqrt{r_1^2+r_0^2-2r_0r_1\cos\theta}$$
$$I_2 \approx \left(\frac{m}{2\pi\hbar^2}\right)^2 \frac{Ae^{ikr}}{r} V_0^2 \iint e^{-i\mathbf{k}\cdot\mathbf{r}_1} \frac{e^{ik\sqrt{r_1^2+r_0^2-2r_0r_1\cos\theta}}}{\sqrt{r_1^2+r_0^2-2r_0r_1\cos\theta}} e^{i\mathbf{k}'\cdot\mathbf{r}_0} d^3\mathbf{r}_0 d^3\mathbf{r}_1$$

We can't really make much headway with this integral without invoking the low energy assumption. In that case, all the exponentials are approximately 1, so we get

$$I_2 \approx \left(\frac{m}{2\pi\hbar^2}\right)^2 \frac{Ae^{ikr}}{r} V_0^2 \iint \frac{d^3\mathbf{r}_0 d^3\mathbf{r}_1}{\sqrt{r_1^2+r_0^2-2r_0r_1\cos\theta}}$$

Doing the $\mathbf{r}_0$ integral first, we have

$$\int \frac{d^3\mathbf{r}_0}{\sqrt{r_1^2+r_0^2-2r_0r_1\cos\theta}} = \int_0^a \int_0^\pi \int_0^{2\pi} \frac{r_0^2\sin\theta\, d\phi d\theta dr_0}{\sqrt{r_1^2+r_0^2-2r_0r_1\cos\theta}}$$
$$= 2\pi \int_0^a \int_0^\pi \frac{r_0^2\sin\theta\, d\theta dr_0}{\sqrt{r_1^2+r_0^2-2r_0r_1\cos\theta}}$$
$$= \frac{2\pi}{r_1} \int_0^a r_0\left[r_0+r_1-|r_0-r_1|\right] dr_0$$
$$= \frac{2\pi}{r_1} \int_0^{r_1} r_0\left[r_0+r_1-(r_1-r_0)\right] dr_0 +$$
$$\frac{2\pi}{r_1} \int_{r_1}^a r_0\left[r_0+r_1-(r_0-r_1)\right] dr_0$$
$$= \frac{4}{3}\pi r_1^2 + 2\pi a^2 - 2\pi r_1^2$$
$$= 2\pi a^2 - \frac{2}{3}\pi r_1^2$$

The integral over $\mathbf{r}_1$ is now easy, and we get

$$I_2 \approx \left(\frac{m}{2\pi\hbar^2}\right)^2 \frac{Ae^{ikr}}{r} V_0^2 \int_0^a \int_0^\pi \int_0^{2\pi} \left(2\pi a^2 - \frac{2}{3}\pi r_1^2\right) r_1^2 \sin\theta\, d\phi d\theta dr_1$$
$$= \frac{Ae^{ikr}}{r} \frac{8m^2V_0^2a^5}{15\hbar^4}$$

The second order correction to the scattering amplitude is the coefficient of $\frac{Ae^{ikr}}{r}$ so the correction is

$$f_2 = \frac{8m^2V_0^2a^5}{15\hbar^4}$$

Combining this with the first order correction taken from Griffiths's Example 11.4 we get

$$f(\theta,\phi) \approx -\frac{2ma^3V_0}{3\hbar^2} + \frac{8m^2V_0^2a^5}{15\hbar^4}$$
$$= -\frac{2ma^3V_0}{3\hbar^2}\left(1 - \frac{4mV_0a^2}{5\hbar^2}\right)$$

17.3.9 Second Order Scattering in Yukawa Potential

GKKG.13.12 2nd order scattering on Yukawa potential

In the 2nd order of perturbation theory, find the scattering amplitude of the Yukawa potential, $U(r) = \frac{\alpha}{r}e^{-r/R}$. Compare $f^{(1)}$ to $f^{(2)}$ for different values of energy and scattering angle.

Solution by Suzuki

(???)
We now study the second-order Born approximation for the Yukawa potential

$$f^{(2)} = -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3\langle\mathbf{k}|\hat{V}\hat{G}_0\left(E_\mathbf{k}+i\varepsilon\right)\hat{V}|\mathbf{k}\rangle$$

with

$$\langle\mathbf{k}|\hat{V}\hat{G}_0\left(E_\mathbf{k}+i\delta\right)\hat{V}|\mathbf{k}\rangle = \int d\mathbf{k}''\,\langle\mathbf{k}'|\,\hat{V}\,|\mathbf{k}''\rangle\,\langle\mathbf{k}''|\,\hat{G}_0\left(E_\mathbf{k}+i\delta\right)|\mathbf{k}''\rangle\,\langle\mathbf{k}''|\,\hat{V}|\mathbf{k}\rangle,$$

$$\langle\mathbf{k}"|\hat{G}_0\left(E_\mathbf{k}+i\delta\right)|\mathbf{k}''\rangle = \langle\mathbf{k}"|\frac{1}{E_\mathbf{k}-\hat{H}+i\delta}\,|\mathbf{k}''\rangle$$

$$= \langle\mathbf{k}''|\,\frac{1}{E_\mathbf{k}-E_{\mathbf{k}^-}+i\delta}\,|\mathbf{k}''\rangle$$

$$= \frac{1}{E_\mathrm{k}-E_{\mathbf{k}^-}+i\varepsilon}$$

$$= \frac{2m}{\hbar^2}\frac{1}{\mathbf{k}^2-\mathbf{k}^{m^2}+i\varepsilon}$$

$$\langle\mathbf{k}|\hat{V}|\mathbf{k}\rangle = \frac{1}{(2\pi)^3}\frac{4\pi V_0}{\mu}\frac{1}{\mu^2+(\mathbf{k}^2-\mathbf{k})^2},$$

$$f^{(2)} = -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3\int d\mathbf{Q}\langle\mathbf{k}|\hat{V}|\mathbf{Q}\rangle\langle\mathbf{Q}|\hat{G}_0\left(E_\mathbf{k}+is\right)|\mathbf{Q}\rangle\langle\mathbf{Q}|\hat{V}|\mathbf{k}\rangle$$

$$= -\frac{1}{4\pi}\left(\frac{2m}{\hbar^2}\right)^2(2\pi)^3\frac{1}{(2\pi)^6}\left(\frac{4\pi V_0}{\mu}\right)^2\int d\mathbf{Q}\frac{1}{\mu^2+(\mathbf{Q}-\mathbf{k}')^2}\frac{1}{\mu^2+(\mathbf{Q}-\mathbf{k})^2}\frac{1}{\mathbf{k}^2-\mathbf{Q}^2+i\delta}$$

$$= \frac{\lambda^2\mu^2}{32\pi^4}\int d\mathbf{Q}\frac{1}{\mu^2+(\mathbf{Q}-\mathbf{k}^2)^2}\frac{1}{\mu^2+(\mathbf{Q}-\mathbf{k})^2}\frac{1}{\mathbf{Q}^2-\mathbf{k}^2-i\delta}$$

where E is a positive small constant. We now calculate the integral M (Dalitz integral) defined by

$$M = \int d\mathbf{Q}\frac{1}{\mu^2+(\mathbf{Q}-\mathbf{k}')^2}\frac{1}{\mu^2+(\mathbf{Q}-\mathbf{k})^2}\frac{1}{\mathbf{Q}^2-\mathbf{k}^2-i\varepsilon}.$$

We use the formula (Feynman integral representation)

$$\int_0^1 dz\frac{1}{[az+b(1-z)]^2} = \frac{1}{ab},$$

In general;

$$\frac{1}{a^mb^z} = \frac{(m+n-1)!}{(m-1)!(n-1)!}\int_0^1\frac{t^{m-1}(1-t)^{n-1}}{[at+b(1-t)]^{m+n}}dt$$

(Feynman, 1949)
Here we also use the notations

$$a = \mu^2 + (\mathbf{Q} - \mathbf{k}')^2, \quad b = \mu^2 + (\mathbf{Q} - \mathbf{k})^2$$

and

$$\begin{aligned} az + b(1-z) &= \left[\mu^2 + (\mathbf{Q} - \mathbf{k}')^2\right] z + \left[\mu^2 + (\mathbf{Q} - \mathbf{k})^2\right](1-z) \\ &= \mu^2 + \left(\mathbf{Q}^2 - 2\mathbf{Q}\cdot\mathbf{k} + \mathbf{k}'^2\right) z + \left(\mathbf{Q}^2 - 2\mathbf{Q}\cdot\mathbf{k} + \mathbf{k}^2\right)(1-z) \\ &= \mu^2 + \mathbf{k}'^2 z + \mathbf{k}^2(1-z) + \mathbf{Q}^2 - 2\mathbf{Q}\cdot[\mathbf{k}'z + \mathbf{k}(1-z)] \\ &= \mu^2 + k^2 + \mathbf{Q}^2 - 2\mathbf{Q}\cdot[\mathbf{k}'z + \mathbf{k}(1-z)] \end{aligned}$$

where

$$\begin{aligned} &\mathbf{q} = \mathbf{k}' - \mathbf{k}, \\ &|\mathbf{k}| = |\mathbf{k}| = k, \qquad \mathbf{k}'\cdot\mathbf{k} = k^2\cos\theta \end{aligned}$$

Thus, we have

$$\begin{aligned} az + b(1-z) &= [\mathbf{Q} - \mathbf{k}'z - \mathbf{k}(1-z)]^2 + \mu^2 + k^2 - [\mathbf{k}'z + \mathbf{k}(1-z)]^2 \\ &= [\mathbf{Q} - \mathbf{k}'z - \mathbf{k}(1-z)]^2 + \mu^2 + k^2 - \mathbf{g}^2 \\ &= (\mathbf{Q} - \mathbf{g})^2 + \tau^2 \end{aligned}$$

For convenience, we use the parameters.

$$\begin{aligned} &\mathbf{g} = \mathbf{k}'z + \mathbf{k}(1-z) = \mathbf{q}z + \mathbf{k}, \\ &\tau^2 = \mu^2 + k^2 - g^2. \\ &g^2 = [\mathbf{k}z + \mathbf{k}'(1-z)]\cdot[\mathbf{k}z + \mathbf{k}'(1-z)] \\ &= \mathbf{k}^2 z^2 + \mathbf{k}'^2(1-z)^2 + 2\mathbf{k}\cdot\mathbf{k}'z(1-z) \\ &= k^2\left[2z^2 - 2z + 1 + 2z(1-z)\cos\theta\right] \\ &= k^2\left[1 - 2z(1-z) + 2z(1-z)\left(1 - 2\sin^2\frac{\theta}{2}\right)\right] \\ &= k^2\left[1 - 4z(1-z)\sin^2\frac{\theta}{2}\right] \end{aligned}$$

$$\mathbf{g}^2 + \tau^2 = \mu^2 + k^2$$

So that, M can be rewritten as

$$\begin{aligned} M &= \int_0^1 dz \int d\mathbf{Q} \frac{1}{4\left[(\mathbf{Q} - \mathbf{g})^2 + \tau^2\right]^2} \frac{1}{\mathbf{Q}^2 - \mathbf{k}^2 - i\varepsilon} \\ &= \int_0^1 dz \int d\mathbf{Q} \frac{1}{\left[(\mathbf{Q} - \mathbf{g})^2 + \tau^2\right]^2} \frac{1}{\mathbf{Q}^2 - \mathbf{k}^2 - i\varepsilon} \end{aligned}$$

and

$$M = \int_0^1 dz L(\mathbf{g}, \boldsymbol{\tau})$$

with

$$\begin{aligned} L(\mathbf{g}, \tau) &= \int d\mathbf{Q} \frac{1}{\left[(\mathbf{Q} - \mathbf{g})^2 + \tau^2\right]^2 \left[\mathbf{Q}^2 - k^2 - i\varepsilon\right]} \\ J(\mathbf{g}, \tau) &= \int d\mathbf{Q} \frac{1}{\left[(\mathbf{Q} - \mathbf{g})^2 + \tau^2\right] \left[\mathbf{Q}^2 - k^2 - i\varepsilon\right]} \end{aligned}$$

and

$$M = -\frac{1}{2\tau}\frac{\partial}{\partial\tau} J(\mathbf{g}, \tau)$$

First, we need to calculate $J(\mathbf{g}, \tau)$. Suppose that the vector $\boldsymbol{g}$ is directed along the Q_z axis. When the angle between the vector $\boldsymbol{Q}$ and $\boldsymbol{g}$ is χ, we have a scalar product as

The scalar product:

$$\mathbf{Q}\cdot\mathbf{g} = Qg\cos\chi$$
$$(\mathbf{Q}-\mathbf{g})^2 = \mathbf{Q}^2 - 2\mathbf{Q}\cdot\mathbf{g} + \mathbf{g}^2 = \mathbf{Q}^2 - 2Qg\cos\chi + \mathbf{g}^2$$

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$$\begin{aligned}
J(\mathbf{g},\tau) &= \int_0^\infty Q^2 dQ \int_0^\pi 2\pi\sin\chi d\chi \frac{1}{[Q^2 - 2Qg\cos\chi + g^2 + \tau^2]\,[Q^2 - k^2 - i\varepsilon]} \\
&= \int_0^\pi 2\pi\sin\chi d\chi \int_0^\infty dQ \frac{Q^2}{[Q^2 - 2Qg\cos\chi + g^2 + \tau^2]\,[Q^2 - k^2 - i\varepsilon]} \\
&= \int_0^\infty \frac{Q^2 dQ}{Q^2 - k^2 - i\delta} \int_0^\pi \frac{2\pi\sin\chi d\chi}{[Q^2 - 2Qg\cos\chi + g^2 + \tau^2]}
\end{aligned}$$

We define the function $F(Q)$ as

$$\begin{aligned}
F(Q) &= \int_0^\pi \frac{2\pi\sin\chi d\chi}{Q^2 + g^2 + \tau^2 - 2Qg\cos\chi} \\
&= \frac{\pi}{gQ}\ln\left(\frac{g^2+\tau^2+2gQ+Q^2}{g^2+\tau^2-2gQ+Q^2}\right)
\end{aligned}$$

$$\begin{aligned}
J(\mathbf{g},\tau) &= \int_0^\pi \frac{Q^2 dQ}{Q^2 - k^2 - i\delta} F(Q) \\
&= \int_0^\infty \frac{Q^2 dQ}{Q^2 - k^2 - i\delta}\left[\frac{\pi}{gQ}\ln\left(\frac{g^2+t^2+2gQ+Q^2}{g^2+t^2-2gQ+Q^2}\right)\right] \\
&= \frac{\pi}{g}\int_0^\infty \frac{QdQ}{Q^2 - k^2 - i\delta}\ln\left(\frac{g^2+t^2+2gQ+Q^2}{g^2+t^2-2gQ+Q^2}\right)
\end{aligned}$$

We note that the integrand of this integral is an even function of Q. This integral can be rewritten as

$$J(\mathbf{g},\tau) = \frac{1}{2}\int_{-\infty}^\infty \frac{Q^2 dQ}{Q^2 - k^2 - i\varepsilon} F(Q).$$

Using the form of $F(Q); F(Q) = \int_0^\pi \frac{2\pi\sin\chi d\chi}{Q^2+g^2+\tau^2-2Qg\cos\chi}$, $J(\mathbf{g},\tau)$ can be obtained as

$$\begin{aligned}
J(\mathbf{g},\tau) &= \frac{1}{2}\int_{-\infty}^\infty \frac{Q^2 dQ}{Q^2 - k^2 - i\delta}\int_0^\pi \frac{2\pi\sin\chi d\chi}{Q^2 + g^2 + t^2 - 2Qg\cos\chi} \\
&= \pi\int_0^\pi \sin\chi d\chi \int_{-\pi}^\infty \frac{Q^2 dQ}{(Q^2 - k^2 - i\delta)\left[(Q - g\cos\chi)^2 + g^2\sin^2\chi + \tau^2\right]}
\end{aligned}$$

Using the Jordan's lemma (the absolute value of the integrand reduces to zero in the limit of $|Q| \to \infty$ in the complex Q-plane), we extend the region of the integral over the upper half of complex plane. Using the Cauchy theorem, we get

$$\begin{aligned}
I &= \int_{-\infty}^\infty \frac{Q^2 dQ}{(Q^2 - k^2 - i\varepsilon)\left[(Q - g\cos\chi)^2 + g^2\sin^2\chi + \tau^2\right]} \\
&= \oint_c \frac{Q^2 dQ}{(Q^2 - k^2 - i\delta)\left[(Q - g\cos\chi)^2 + g^2\sin^2\chi + \tau^2\right]} \\
&= \oint_c \frac{Q^2 dQ}{(Q - Q_1)(Q - Q_2)(Q - Q_3)(Q - Q_4)} \\
&= 2\pi\left[\mathrm{Re}\, s\,(Q = Q_1) + \mathrm{Re}\, s\,(Q = Q_3)\right]
\end{aligned}$$

$$\begin{aligned}
\operatorname{Re} s(Q=Q_1) &= \lim_{Q\to 2} \frac{Q^2\,(Q-Q_1)}{(Q-Q_1)\,(Q-Q_2)\,(Q-Q_3)\,(Q-Q_4)} \\
&= \lim_{Q\to Q} \frac{Q^2}{(Q-Q_2)\,(Q-Q_3)\,(Q-Q_4)} \\
&= \frac{Q_1^2}{(Q_1-Q_2)\,(Q_4-Q_3)\,(Q_4-Q_4)} \\
&= \frac{k^3}{2}\frac{1}{k^2+g^2+\tau^2-2g\cos\chi} \\
&= \frac{k^3}{2}\frac{1}{k^2+\mu^2+k^2-2g\cos\chi}
\end{aligned}$$

where

$$\begin{aligned}
g^2+\tau^2 &= \mu^2+k^2, \\
\operatorname{Re} s(Q=Q_3) &= \lim_{Q\to \varrho} \frac{Q^2\,(Q-Q_3)}{(Q_1-Q_1)\,(Q-Q_2)\,(Q-Q_3)\,(Q-Q_4)} \\
&= \lim_{Q\to \Theta} \frac{Q^2}{(Q-Q_1)\,(Q-Q_2)\,(Q-Q_4)} \\
&= \frac{Q_3^2}{(Q_3-Q_1)\,(Q_3-Q_2)\,(Q_3-Q_4)} \\
&= \frac{(g\cos\chi+i\alpha)^2}{2i\alpha(g\cos\chi+i\alpha+k)(g\cos\chi+i\alpha-k)} \\
&= \frac{(g\cos\chi+i\alpha)^2}{2i\alpha\left[(g\cos\chi+i\alpha)^2-k^2\right]}
\end{aligned}$$

and

$$\begin{aligned}
\operatorname{Re} s(Q=Q_3) &= \frac{k^2}{2k}\frac{1}{(k-g\cos\chi)^2+g^2\sin^2\chi+\tau^2} \\
&= \frac{k}{2}\frac{1}{k^2+g^2+\tau^2-2kg\cos\chi}
\end{aligned}$$

Where we define α as

$$\alpha = \sqrt{g^2\sin^2\chi+\tau^2}$$

We now calculate

$$\begin{aligned}
J(\mathbf{g},\tau) &= 2\pi^2 i \int_0^\pi \sin\chi d\chi \left[\operatorname{Res}(Q=Q_1)+\operatorname{Res}(Q=Q_3)\right. \\
&= J_1+J_3
\end{aligned}$$

where

$$\begin{aligned}
J_1 &= 2\pi^2 i \int_0^\pi \sin\chi d\chi \left[\operatorname{Res}(Q=Q_1)\right] \\
&= 2\pi^2 i \int_0^\pi \sin\chi d\chi \frac{(g\cos\chi+i\alpha)^2}{2i\alpha\left[(g\cos\chi+i\alpha)^2-k^2\right]} \\
&= \pi^2 \int_0^\pi \sin\chi d\chi \frac{(g\cos\chi+i\alpha)^2}{\alpha\left[(g\cos\chi+i\alpha)^2-k^2\right]}
\end{aligned}$$

For simplicity, we choose a variable,

$$x = g\cos\chi+i\alpha = g\cos\chi+i\sqrt{g^2\sin^2\chi+\tau^2}$$

and

$$
\begin{aligned}
dx &= \left[-g\sin\chi + i\frac{g^2\sin\chi\cos\chi}{\sqrt{g^2\sin^2\chi+\tau^2}} \right] d\chi \\
&= \frac{ig\sin\chi}{\sqrt{g^2\sin^2\chi+\tau^2}} \left[i\sqrt{g^2\sin^2\chi+\tau^2} + g\cos\chi \right] d\chi \\
&= \frac{ig\sin\chi}{\sqrt{g^2\sin^2\chi+r^2}} (g\cos\chi + i\alpha) d\chi \\
&= \frac{ig\sin\chi}{\alpha} x d\chi
\end{aligned}
$$

$$
\sin\chi d\chi = \frac{\alpha}{ig}\frac{dx}{x}
$$

Then we have

$$
\begin{aligned}
J_1 &= \pi^2 \int_{g^{+iz}}^{-g+it} \frac{\alpha dx}{igx} \frac{x^2}{\alpha\left(x^2-k^2\right)} \\
&= \frac{i\pi^2}{g} \int_{-g^{+ir}}^{t^{+ir}} \frac{xdx}{x^2-k^2} \\
&= \frac{i\pi^2}{2g} \int_{-g^{+ir}}^{g^{+ir}} \left(\frac{1}{x-k} + \frac{1}{x+k} \right) dx \\
&= \frac{i\pi^2}{2g} \ln \frac{(i\tau-k+g)(i\tau+k+g)}{(i\tau-k-g)(i\tau+k-g)}
\end{aligned}
$$

We also calculate the integral J_3

$$
\begin{aligned}
J_3 &= 2\pi^2 i \int_0^\pi \sin\chi d\chi \left[\mathrm{Res}\left(Q=Q_3\right) \right] \\
&= 2\pi^2 i \int_0^\pi \sin\chi d\chi \frac{k}{2} \frac{1}{k^2+g^2+\tau^2-2kg\cos\chi} \\
&= k\pi^2 i \int_0^\pi \frac{\sin\chi d\chi}{k^2+g^2+\tau^2-2kg\cos\chi} \\
&= \frac{\pi^2 i}{2g} \ln \frac{(k+g)^2+\tau^2}{(k-g)^2+\tau^2}
\end{aligned}
$$

Thus, we have

$$
\begin{aligned}
J &= J_1 + J_3 \\
&= \frac{\pi^2 i}{2g} \left[\ln \frac{(i\tau+k+g)(i\tau-k-g)}{(i\tau+k-g)(i\tau-k+g)} + \ln \frac{(i\tau-k+g)(i\tau+k+g)}{(i\tau-k-g)(i\tau+k-g)} \right] \\
&= \frac{\pi^2 i}{g} \ln \frac{(i\tau+k+g)}{(i\tau+k-g)}
\end{aligned}
$$

M is defined by

$$
M = -\frac{1}{2\tau}\frac{\partial}{\partial\tau} J(\mathbf{g},\tau) = -\frac{\pi^2}{\tau} \frac{1}{k^2-g^2-\tau^2+2i\tau k}.
$$

The scattering amplitude in the second order Born approximation is

$$
\begin{aligned}
f^{(2)} &= \frac{1}{32\pi^2}\lambda^2\mu^2 \int_0^1 M dz \\
&= -\frac{1}{32\pi^2}\lambda^2\mu^2 \int_0^1 \frac{dz}{\tau\left(k^2 - g^2 - \tau^2 + 2i\tau k\right)} \\
&= -\frac{1}{32\pi^2}\lambda^2\mu^2 \int_0^1 \frac{dz}{\tau\left(-\mu^2 + 2i\tau k\right)}
\end{aligned}
$$

where

$$
g^2 + \tau^2 = k^2 + \mu^2,
$$

and

$$
\begin{aligned}
\tau^2 &= \mu^2 + k^2 - g^2 \\
&= \mu^2 + 4k^2 \sin^2\frac{\theta}{2} z(1-z) \\
&= \mu^2 + q^2 z(1-z)
\end{aligned}
$$

Using the separation of the real part and imaginary part of the integrand

$$
\begin{aligned}
\frac{1}{\tau\left(-\mu^2 + 2i\tau k\right)} &= \frac{\left(-\mu^2 - 2i\tau k\right)}{\tau\left(\mu^4 + 4\tau^2 k^2\right)} \\
&= -\frac{\mu^2}{\tau\left(\mu^4 + 4\tau^2 k^2\right)} + \frac{-2ik}{\left(\mu^4 + 4\tau^2 k^2\right)}
\end{aligned}
$$

(a) Imaginary part $\mathrm{Im}\left[f^{(2)}\right]$
We have the imaginary part,

$$
\begin{aligned}
\mathrm{Im}\left[f^{(2)}\right] &= -\frac{1}{32\pi^2}\lambda^2\mu^2 \int_0^1 \frac{-2k dz}{\mu^4 + 4\tau^2 k^2} \\
&= \frac{1}{16\pi^2} k\lambda^2\mu^2 \int_0^1 \frac{dz}{\mu^4 + 4\tau^2 k^2} \\
&= \frac{1}{16\pi^2} k\lambda^2\mu^2 \int_0^1 \frac{dz}{\mu^4 + 4\mu^2 k^2 + 4k^2 q^2 z(1-z)} \\
&= \frac{1}{16\pi^2} k\lambda^2\mu^2 \frac{\ln\left(\frac{\sqrt{\mu^4 + k^2q^2 + 4\mu^2k^2} + kq}{\sqrt{\mu^4 + k^2q^2 + 4\mu^2k^2} - kq}\right)}{2kq\sqrt{\mu^4 + k^2q^2 + 4\mu^2k^2}}
\end{aligned}
$$

or

$$
\mathrm{Im}\left[f^{(2)}\right] = \frac{1}{32\pi^2}\frac{\lambda^2\mu^2}{q}\frac{\ln\left(\frac{\sqrt{\mu^4 + k^2q^2 + 4\mu^2k^2} + kq}{\sqrt{\mu^4 + k^2q^2 + 4\mu^2k^2} - kq}\right)}{\sqrt{\mu^4 + k^2q^2 + 4\mu^2k^2}}
$$

where the integral is calculated by Mathematica

$$
I_{BC} = \int_0^1 \frac{dz}{\mu^4 + 4\mu^2 k^2 + 4k^2 q^2 z(1-z)} = \frac{\ln\left(\frac{\sqrt{\mu^4 + k^2q^2 + 4\mu^2k^2} + kq}{\sqrt{\mu^4 + k^2q^2 + 4\mu^2k^2} - kq}\right)}{2kq\sqrt{\mu^4 + k^2q^2 + 4\mu^2k^2}}
$$

Note that in the limit of $q \to 0$, we get

$$
\lim_{q\to 0} I_{BM} = \frac{1}{\mu^2}\frac{1}{4k^2 + \mu^2},
$$

leading to the relation

$$\mathrm{Im}\left[f^{(2)}(0)\right] = \frac{\lambda^2}{16\pi^2} k \frac{1}{4k^2+\mu^2}$$

(b) Real part $\mathrm{Re}\left[f^{(2)}\right]$
Next, we calculate the real part,

$$\begin{aligned}\mathrm{Re}\left[f^{(2)}\right] &= \frac{1}{32\pi^2}\lambda^2\mu^2 \int_0^1 \frac{\mu^2 dz}{\tau\left(\mu^4+4r^2k^2\right)} \\ &= \frac{1}{32\pi^2}\mu^4\lambda^2 \int_0^1 \frac{dz}{\sqrt{\mu^2+q^2z(1-z)}\left[\mu^4+4\mu^2k^2+4k^2q^2z(1-z)\right]}\end{aligned}$$

where the solution of this integral is also obtained using the Mathematica 26

$$\begin{aligned}I_R &= \int_0^1 \frac{dz}{\sqrt{\mu^2+q^2z(1-z)}\left[\mu^4+4\mu^2k^2+4k^2q^2z(1-z)\right]} \\ &= \frac{1}{q\mu^2\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}\left[\mathrm{Arctan}\,\frac{k\left(q^2+4\mu^2\right)+q\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{2\mu^3}\right. \\ &\left. -\,\mathrm{Arctan}\,\frac{k\left(q^2+4\mu^2\right)-q\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{2\mu^3}\right]\end{aligned}$$

and

$$\lim_{q\to 0} I_n = \frac{1}{\mu^3}\frac{1}{4k^2+\mu^2}.$$

Thus, we have

$$\begin{aligned}\mathrm{Re}\left[f^{(2)}\right] =& \frac{1}{32\pi^2}\mu^4\lambda^2\frac{1}{q\mu^2\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}} \\ &\times \mathrm{Arctan}\,\frac{k\left(q^2+4\mu^2\right)+q\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{2\mu^3} \\ &-\,\mathrm{Arctan}\,\frac{k\left(q^2+4\mu^2\right)-q\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{2\mu^3}\Bigg]\end{aligned}$$

We also have simpler expression as

$$\begin{aligned}\mathrm{Re}\left[f^{(2)}\right] =& \frac{1}{32\pi^2}\frac{\lambda^2\mu^2}{q}\frac{1}{\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}} \\ &\mathrm{Arctan}\left[\frac{q\mu\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{\mu^4+k^2\left(q^2+4\mu^2\right)-\frac{q^2\mu^2}{4}}\right]\end{aligned}$$

(see the note for this derivation)
We note that 27

$$\lim_{q\to 0}\frac{1}{q}\,\mathrm{Arctan}\left[\frac{q\mu}{\sqrt{\mu^4+4k^24\mu^2}}\right] = \frac{\mu}{\sqrt{\mu^2+4k^2}}$$

Using this relation, we have

$$\mathrm{Re}\left[f^{(2)}(0)\right] = \frac{1}{32\pi^2}\lambda^2\mu\frac{1}{\mu^2+4k^2},$$

at $q=0$.
(Note)) Simplification of the expression of $\mathrm{Re}\left[f^{(2)}\right]$ We now simplify the expression of $\mathrm{Re}\left[f^{(2)}\right]$ using simple trigonometry. 29

$$
\begin{aligned}
A &= \operatorname{Arctan} \frac{k\left(q^2+4\mu^2\right)+q\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{2\mu^3} \\
&\quad - \operatorname{Arctan} \frac{k\left(q^2+4\mu^2\right)-q\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{2\mu^3} \\
&= \alpha - \beta
\end{aligned}
$$

where we use α and β as

$$
\begin{aligned}
\tan\alpha &= \frac{k\left(q^2+4\mu^2\right)+q\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{2\mu^3}, \\
\tan\beta &= \frac{k\left(q^2+4\mu^2\right)-q\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{2\mu^3}
\end{aligned}
$$

We note that

$$
\tan(\alpha-\beta) = \frac{\tan\alpha-\tan\beta}{1+\tan\alpha\tan\beta}.
$$

Then, we get

$$
\begin{aligned}
\tan\alpha - \tan\beta &= \frac{q}{\mu^3}\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}, \\
1+\tan\alpha\tan\beta &= 1+\left[\frac{k\left(q^2+4\mu^2\right)+q\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{2\mu^3}\right] \\
&\quad \times \left[\frac{k\left(q^2+4\mu^2\right)-q\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{2\mu^3}\right] \\
&= 1+\frac{1}{4\mu^6}\left[k^2\left(q^2+4\mu^2\right)^2-\left(q^2\mu^4+q^4k^2+4k^2q^2\mu^2\right)\right] \\
&= 1+\frac{1}{4\mu^6}\left[k^2\left(q^4+8q^2\mu^2+16\mu^4\right)-\left(q^2\mu^4+q^4k^2+4k^2q^2\mu^2\right)\right] \\
&= 1+\frac{1}{4\mu^4}\left[4k^2\left(q^2+4\mu^2\right)-q^2\mu^2\right] \\
&= \frac{1}{\mu^4}\left[\mu^4+k^2\left(q^2+4\mu^2\right)\right]-\frac{q^2}{4\mu^2}
\end{aligned}
$$

Thus, we have

$$
\begin{aligned}
\tan(\alpha-\beta) &= \frac{\frac{q}{\mu^3}\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{\frac{1}{\mu^4}\left[\mu^4+k^2\left(q^2+4\mu^2\right)\right]-\frac{q^2}{4\mu^2}} \\
&= \frac{q\mu\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{\left[\mu^4+k^2\left(q^2+4\mu^2\right)\right]-\frac{q^2\mu^2}{4}}
\end{aligned}
$$

or

$$
\alpha-\beta = \operatorname{Arctan}\left[\frac{q\mu\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{\left[\mu^4+k^2\left(q^2+4\mu^2\right)\right]-\frac{q^2\mu^2}{4}}\right]
$$

6. Optical theorem
The scattering amplitude up to the second order, is

$$
f = f^{(1)} + f^{(2)} =
$$

At $q=0$, we get the scattering amplitude as

$$
f^{(1)} = -\frac{\lambda}{4\pi}\mu\frac{1}{\mu^2} = -\frac{\lambda}{4\pi}\frac{1}{\mu}
$$

and

$$\begin{aligned} f^{(2)} &= \frac{\lambda^2}{32\pi^2}\frac{\mu}{\mu^2+4k^2} + i\frac{1}{16}\lambda^2\left(\frac{k}{\mu^2+4k^2}\right) \\ &= \frac{\lambda^2}{32\pi^2}\left(\frac{\mu+2ik}{\mu^2+4k^2}\right) \\ &= \frac{\lambda^2}{32\pi^2}\frac{1}{\mu-2ik} \end{aligned}$$

If the Born approximation is to be reliable, we must certainly have the condition

$$\frac{\left|f^{(2)}\right|}{\left|f^{(1)}\right|} * 1$$

For the forward scattering ($q = 0$), we gave

$$\frac{\left|f^{(2)}\right|}{\left|f^{(1)}\right|} = \frac{\frac{\lambda^2}{32\pi^2}\frac{1}{\sqrt{\mu^2+4k^2}}}{\frac{\lambda}{4\pi\mu}} = \frac{\lambda}{8\pi}\frac{\mu}{\sqrt{\mu^2+4k^2}} * 1$$

When $k > \mu$ (high energy)

$$\frac{\left|f^{(2)}\right|}{\left|f^{(1)}\right|} = \frac{\lambda}{16\pi}\frac{\mu}{k} * 1$$

The condition steadily improved as k increases. When $k\&\mu$ (low energy, $k = 0$),

$$\frac{\left|f^{(2)}\right|}{\left|f^{(1)}\right|} = \frac{\lambda}{8\pi} \approx 1$$

By taking into account of the second order $\operatorname{lm}\left[f^{(2)}(0)\right]$, we confirm that the optical theorem is valid such that

$$\begin{aligned} \frac{4\pi}{k}\operatorname{lm}[f(0)] &= \frac{4\pi}{k}\operatorname{Im}\left[f^{(1)}(0) + f^{(2)}(0)\right] \\ &= \frac{4\pi}{k}\operatorname{Im}\left[f^{(2)}(0)\right] \\ &= \frac{\lambda^2}{4\pi}\frac{1}{\mu^2+4k^2} \\ &= \sigma^{(1)} \end{aligned}$$

where

$$\sigma_{\mathrm{sa}}{}^{(1)} = \frac{\lambda^2}{4\pi}\frac{1}{\mu^2+4k^2}$$

We note that the differential cross section is

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= |f|^2 \\ &= |f^{(1)} + \operatorname{Re}\left[f^{(2)}\right] + \operatorname{Im}\left[f^{(2)}\right|^2 \\ &= \left(f^{(1)} + \operatorname{Re}\left[f^{(2)}\right]\right)^2 + \left(\operatorname{Im}\left[f^{(2)}\right]\right)^2 \\ f^{(1)} &= -\frac{\lambda\mu}{4\pi}\frac{1}{\mu^2+q^2} \\ \operatorname{Re}\left[f^{(2)}\right] &= \frac{1}{32\pi^2}\frac{\lambda^2\mu^2}{q}\frac{1}{\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}} \\ &\quad \operatorname{Arctan}\left[\frac{q\mu\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{\mu^4+k^2\left(q^2+4\mu^2\right)-\frac{q^2\mu^2}{4}}\right] \end{aligned}$$

and

$$\operatorname{Im}\left[f^{22}\right] = \frac{1}{32\pi^2}\frac{\lambda^2\mu^2}{q}\frac{\ln\left(\frac{\sqrt{\mu^4+k^2(q^2+4\mu)}+kq}{\sqrt{\mu^4+k^2(q^2+4\mu^2)}-kq}\right)}{\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}$$

So that, we have the final form

$$\begin{aligned}
f =& f^{(1)} + f^{(2)} \\
=& -\frac{\lambda\mu}{4\pi}\frac{1}{\mu^2+q^2} \\
&+\frac{1}{32\pi^2}\frac{\lambda^2\mu^2}{q}\left[\frac{1}{\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}\operatorname{Arctan}\left[\frac{q\mu\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}{\mu^4+k^2\left(q^2+4\mu^2\right)-\frac{q^2\mu^2}{4}}\right]\right. \\
&\left.+i\frac{\ln\left(\frac{\sqrt{\mu^4+k^2(q^2+4\mu^2)}+kq}{\sqrt{\mu^4+k^2(q^2+4\mu^2)}-kq}\right)}{\sqrt{\mu^4+k^2\left(q^2+4\mu^2\right)}}\right]
\end{aligned}$$

7. Validity of the Born approximation (another approach); direct calculation The validity for the Born approximation is satisfied under the condition

$$\left|\frac{m}{2\pi\hbar^2}\int d\mathbf{r}\frac{e^\star}{r}V(r)\right| \ll 1$$

$$\left|\frac{m}{2\pi\hbar^2}\int d\mathbf{r}\frac{e^*}{r}\frac{V_0}{\mu r}e^{-\mu p}\right| \ll 1$$

We note that

$$\begin{aligned}
\int d\mathbf{r}\frac{e^{dr}}{r}\frac{V_0}{\mu r}e^{-\mu r} &= 4\pi\int_0^\pi dr r^2\frac{e^{jr}}{r}\frac{V_0}{\mu r}e^{-\mu r} \\
&= 4\pi\frac{V_0}{\mu}\int_0^\pi dr e^{(ik-\mu)r} \\
&= 4\pi\frac{V_0}{\mu}\frac{1}{\mu-ik} \\
\left|\frac{m}{2\pi\hbar^2}4\pi\frac{V_0}{\mu}\frac{1}{\mu-ik}\right| &= \frac{2m}{\hbar^2}\frac{V_0}{\mu}\frac{1}{\sqrt{\mu^2+k^2}} \ll 1
\end{aligned}$$

(a) Low energy limit ($k \ll \mu$)

$$\frac{2m}{\hbar^2}\frac{V_0}{\mu^2} \ll 1 \quad |\lambda| \ll 4\pi$$

(b) High energy limit ($k \gg \mu$)

$$\frac{2m}{h^2}\frac{V_0}{\mu k} \ll 1 \quad |\lambda| \ll 4\pi\frac{k}{\mu}$$

The inequality becomes easier to satisfy to satisfy as k increases, implying that the Born approximation becomes much accurate at high incident particle energy. ((Note)) Scattering length a The scattering length a is defined by

$$a = \frac{\beta}{\mu},$$

as will be derived later, with $\beta = \frac{4\pi}{\lambda} = \frac{2mV_0}{\hbar^2\mu^2}$. The condition for the scattering for the high energy limit (as described above) is

$$|\lambda| \ll 4\pi\frac{k}{\mu}$$

This condition can be rewritten as

$$ka > 1$$

The de Broglie wavelength Λ is related as the wave number as

$$\Lambda = \frac{2\pi}{k}$$

So that, the condition is also expressed as

$$a \geqslant \frac{\Lambda}{2\pi}.$$

The de Broglie wavelength Λ is much shorter than the scattering length a. 8. Partial phase shift

The Born approximation is a good approximation for the high energy incident particle, but is not so for the low energy incident particle.

$$f(E,q) = \sum_{i=0}^{\pi}(2l+1)f_i(E)P(\cos\theta)$$

$$f_i(E) = \frac{1}{2}\int_{-1}^{1} dz P_i(z) f(E,q)$$

$$z = \cos\theta$$

$1 - \cos\theta = \frac{q^2}{2k^2} = \frac{\hbar^2 q^2}{4mE}$,

$$\begin{aligned} f^{(1)} &= -\frac{\lambda\mu}{4\pi}\frac{1}{\mu^2+q^2} \\ &= -\frac{\lambda\mu}{4\pi}\frac{1}{\mu^2+2k^2(1-\cos\theta)} \\ &= -\frac{\lambda\mu}{4\pi}\frac{1}{\mu^2+2k^2(1-z)} \\ &= -\frac{\lambda\mu}{4\pi}\frac{1}{\mu^2+\frac{4mE}{\hbar^2}(1-z)} \end{aligned}$$

For $l = 0$ (s-wave)

$$\begin{aligned} f_0(E) &= \frac{1}{2}\int_{-1}^{1} dz f^{(1)}(E,q) \\ &= \frac{-\lambda\mu}{8\pi}\int_{-1}^{1} dz \frac{1}{\mu^2+\frac{4mE}{\hbar^2}(1-z)} \\ &= \frac{-\lambda\mu}{8\pi}\frac{\hbar^2}{4mE}\ln\left[\mu^2+\frac{4mE}{\hbar^2}(1-z)\right]\Big|_{-1}^{1} \\ &= \frac{\lambda\mu\hbar^2}{32\pi mE}\ln\left[\frac{\mu^2}{\mu^2+\frac{8mE}{\hbar^2}}\right] \\ &= \frac{\gamma}{4E}\ln\left[\frac{\mu^2}{\mu^2+\frac{8mE}{\hbar^2}}\right] \end{aligned}$$

where

$$\gamma = \frac{V_0}{\mu}$$

which has the expected branch point at $E = -\frac{\hbar^2\mu^2}{8m}$. Thus, while the scattering amplitude $f^{(1)}$ has no branch points, the partial amplitude does. This illustrates (which is, in fact, true of all partial waves) that the left-hand branch cut is introduced into the partial-wave amplitude in the process of making the projection (Taylor). 9. Phase shift analysis using the Heine expansion

Using the Heine expansion,

$$\frac{1}{x-\cos\theta} = \sum_{l=0}^{\pi}(2l+1)Q_l(x)P_i(\cos\theta)$$

we get the expansion of $f^{(1)}$ as

$$f^{(1)} = -\frac{2mV_0}{\hbar^2\mu}\frac{1}{\mu^2+4k^2\sin^2\frac{\theta}{2}} = -\frac{2mV_0}{\hbar^2\mu}\frac{1}{\mu^2+2k^2(1-\cos\theta)} = -\frac{mV_0}{\hbar^2\mu k^2}\frac{1}{1+\frac{\mu^2}{2k^2}-\cos\theta} \equiv -\frac{mV_0}{\hbar^2\mu k^2}\frac{1}{x-\cos\theta};$$

$x := 1 + \frac{\mu^2}{2k^2}$

$$f^{(1)} = -\frac{mV_0}{\hbar^2\mu k^2}\frac{1}{x-\cos\theta} \qquad = -\frac{mV_0}{\hbar^2\mu k^2}\sum_{l=0}^{\infty}(2l+1)Q_l(x)P_l(\cos\theta) = \sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\cos\theta)$$

$$f_l(k) = -\frac{mV_0}{\hbar^2\mu k^2}Q_l(x)$$

Solution by GKKG

(ниже компактное решение, над которым нужно думать много, вообще)
For the Yukawa potential,

$$f^{(1)}(q) \equiv f^B(q) = -\frac{2m\alpha R^2}{\hbar^2\left(1+q^2R^2\right)}, \quad \mathbf{q} = \mathbf{k} - \mathbf{k}_0 \tag{1}$$

and according to Eq. (2) from Problem 13.10, in the 2nd order of perturbation theory we have

$$f^{(2)}\left(\mathbf{k}_0, \mathbf{k}_0\right) = \frac{2m^2\alpha^2R^4}{\pi^2\hbar^4}\int \frac{d^3\kappa}{\left[1+R^2\left(\mathbf{k}_0-\boldsymbol{\kappa}\right)^2\right]\left[1+R^2(\mathbf{k}-\boldsymbol{\kappa})^2\right]\left(\kappa^2-k_0^2-i\varepsilon\right)} \tag{2}$$

Using relation (with $k^2 = k_0^2$)

$$\frac{1}{1+R^2\left(\mathbf{k}_0-\boldsymbol{\kappa}\right)^2}\cdot\frac{1}{1+R^2(\mathbf{k}-\boldsymbol{\kappa})^2} = \int_0^1 \frac{d\xi}{\left\{1+k^2R^2+\kappa^2R^2-2R^2\kappa\left[\mathbf{k}_0\xi+(1-\xi)\mathbf{k}\right]\right\}^2}$$

in Eq. (2) it is easy to perform integration over the angles $\left(d^3\kappa = \kappa^2 d\kappa d\Omega\right)$, and obtain

$$f^{(2)}\left(\mathbf{k}_0, \mathbf{k}_0\right) = \frac{4m^2\alpha^2R^4}{\pi\hbar^4}\int_0^1\int_{-\infty}^{\infty}\frac{\kappa^2}{\kappa^2-k^2-i\varepsilon}K(k,q,\kappa,\xi)d\kappa d\xi \tag{3}$$

where

$$K = \left\{\left(1+k^2R^2+\kappa^2R^2\right)^2 - 4\kappa^2R^4\left[k^2-\xi(1-\xi)q^2\right]\right\}^{-1} \tag{4}$$

Taking into account the parity of the function under the integral, the integration over the variable κ may be extended to the entire axis.

Equation (4) for K could be transformed to

$$K = \frac{1}{(\kappa R-\alpha_1)(\kappa R-\alpha_2)(\kappa R-\alpha_3)(\kappa R-\alpha_4)}$$

This function, considered as a function of the complex variable κ, is (as is the entire expression under the integral in Eq. (3)) meromorphic, and has only simple poles at the points $\kappa_n = \alpha_n/R$. We have

$$\alpha_1 \equiv \alpha = \sqrt{k^2R^2-\xi(1-\xi)q^2R^2} + i\sqrt{1+\xi(1-\xi)q^2R^2}$$

(since $0 \le \xi \le 1$ and $q^2 \le 4k^2$, then both radicals are real and positive) and $\alpha_2 = \alpha^*$, $\alpha_3 = -\alpha, \alpha_4 = -\alpha^*$.

Now, in Eq. (3), it is easy to perform an integration over κ using residues, closing the integration contour into the upper half-plane of the complex variable κ.

The positions of the poles are shown in Fig. 13.2. A contribution to the integral in Eq. (3) from the pole at the point $\kappa = k + i\varepsilon$ is

$$I_1(\xi) = \frac{i\pi k}{1+4k^2R^2+4k^2q^2R^4\xi(1-\xi)}$$

This part of the integral is imaginary. The contributions from the poles located at the points $\kappa = \alpha_1/R$ and $\kappa = \alpha_4/R$ are real and equal to

$$I_2(\xi) = \frac{\pi}{2R\sqrt{1+q^2R^2\xi(1-\xi)}\left[1+4k^2R^2\left(1+q^2R^2\xi(1-\xi)\right)\right]}$$

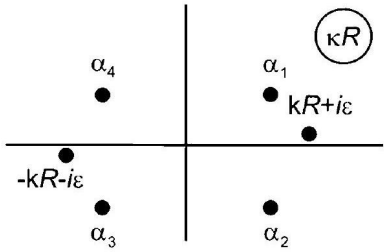


Fig. 13.2
Finally, performing an integration over the variable ξ in

$$f^{(2)}(\mathbf{k},\mathbf{k}_0)=\frac{4m^2\alpha^2R^4}{\pi\hbar^4}\int\limits_0^1\left[I_1(\xi)+I_2(\xi)\right]d\xi$$

we obtain the final expression for the scattering amplitude of the Yukawa potential in second-order perturbation theory:

$$f^{(2)}(\mathbf{k},\mathbf{k}_0)=\frac{2m^2\alpha^2R^3}{\hbar^4}\left\{\frac{2\arctan(qR/2\sqrt{\Delta(k,q)})}{qR\sqrt{\Delta(k,q)}}+\frac{i}{qR\sqrt{\Delta(k,q)}}\ln\frac{\sqrt{\Delta(k,q)}+kqR^2}{\sqrt{\Delta(k,q)}-kqR^2}\right\}\tag{5}$$

where

$$\Delta(k,q)=1+k^2R^2\left(4+q^2R^2\right)$$

Let us discuss these results. We first note that calculating the imaginary part of the amplitude in second-order perturbation theory for $\theta=0$ (here also $q=0$) and using the optical theorem, Eq. (XIII.11), we can find the total scattering cross-section in the Born approximation. The result obtained coincides, of course, with the calculation of cross-section by the equation $\sigma_B=\int\left(f^B\right)^2d\Omega$. See Problem 13.1 a.

It is interesting to compare $\operatorname{Im}f^{(2)}$ and $\operatorname{Re}f^{(2)}$ with each other and with the amplitude of the first approximation for different values of the energy and the scattering angle. In the case of slow particles, when $kR\ll1$, according to Eqs. (5) and (1), we obtain

$$\frac{\operatorname{Im}f^{(2)}}{\operatorname{Re}f^{(2)}}\approx2kR\ll1,\quad\left|\frac{f^{(2)}}{f^{(1)}}\right|\approx\frac{m\alpha R}{\hbar^2}$$

Taking into account the optical theorem, we can conclude that the smallness of the ratio $\operatorname{Im}f^{(2)}/\operatorname{Re}f^{(2)}$ (for $kR\ll1$) is a general result for fairly arbitrary short-range potentials. The smallness of $\left|f^{(2)}/f^{(1)}\right|$ assumes fulfilment of the condition $m\alpha R/\hbar^2\ll1$, which ensures applicability of the Born approximation (see Eq. (XIII.7); for the Yukawa potential, $U_0\sim\alpha/R$). These estimates are also useful for particles of "moderate" energy, $kR\sim1$, but in this case, $\operatorname{Im}f^{(2)}$ and $\operatorname{Re}f^{(2)}$ are quantities of the same order for an arbitrary scattering angle.

Let us consider the case of fast particles, $kR\gg1$. For small scattering angles, when $qR\lesssim1$ (this domain provides a dominant contribution into the total scattering cross-section), we find

$$\frac{\operatorname{Im}f^{(2)}}{\operatorname{Re}f^{(2)}}\sim kR\gg1,\quad\left|\frac{f^{(2)}}{f^{(1)}}\right|\sim\frac{m\alpha}{\hbar^2k}$$

The smallness of $\operatorname{Re}f^{(2)}$ in comparison to $\operatorname{Im}f^{(2)}$ is a general result (see Problem 13.14), while the condition $\left|f^{(2)}/f^{(1)}\right|\ll1$, as expected, assumes that the applicability condition of the Born approximation for fast particles is satisfied, namely the second of conditions (XIII.7). The obtained estimates remain valid for larger value of qR. (Here, some specific properties of the Yukawa potential manifest themselves, in particular, a power-law decrease of $\tilde{U}(q)$ for $q\to\infty$; compare to result of the previous problem.)

Sakurai-6.5 Yukawa scattering

A spinless particle is scattered by a weak Yukawa potential

$$V=\frac{V_0e^{-\mu r}}{\mu r}$$

where $\mu>0$ but V_0 can be positive or negative. It was shown in the text that the first-order Born amplitude is given by

$$f^{(1)}(\theta)=-\frac{2mV_0}{\hbar^2\mu}\frac{1}{[2k^2(1-\cos\theta)+\mu^2]}.$$

(a) Using $f^{(1)}(\theta)$ and assuming $|\delta_l| \ll 1$, obtain an expression for δ_l in terms of a Legendre function of the second kind,

$$Q_l(\zeta) = \frac{1}{2}\int_{-1}^{1} \frac{P_l(\zeta')}{\zeta - \zeta'} d\zeta'$$

(b) Use the expansion formula

$$Q_l(\zeta) = \frac{l!}{1\cdot 3\cdot 5\cdots(2l+1)} \times \left\{ \frac{1}{\zeta^{l+1}} + \frac{(l+1)(l+2)}{2(2l+3)}\frac{1}{\zeta^{l+3}} + \frac{(l+1)(l+2)(l+3)(l+4)}{2\cdot 4\cdot(2l+3)(2l+5)}\frac{1}{\zeta^{l+5}} + \cdots \right\} \quad (|\zeta| > 1)$$

to prove each assertion. (i) δ_l is negative (positive) when the potential is repulsive (attractive). (ii) When the de Broglie wavelength is much longer than the range of the potential, δ_l is proportional to k^{2l+1}. Find the proportionality constant.

Solution by Suzuki

Yukawa potential

$$V(r) = \frac{V_0}{\mu\mu} e^{-\mu r}.$$

The first Born approximation

$$f^{(1)}(\theta) = -\frac{2mV_0}{\hbar^2\mu}\frac{1}{q^2+\mu^2},$$

where

$$\boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k}'$$

$$q^2 = k^2 + k'^2 - 2kk'\cos\theta = 2k^2(1-\cos\theta)$$

where the angle between the vctors $\boldsymbol{k}$ and $\boldsymbol{k}'$ is $\theta.k' = k$ (b)
The scattering amplitude $f(\theta)$ can be expanded in terms of the phase shift δ_l as

$$f(\theta) = \sum_{l'=0}^{\infty} (2l'+1)\, f_{l'}(k) P_{l'}(\cos\theta)$$

Note that

$$I = \int_{-1}^{1} d(\cos\theta) P_l(\cos\theta) f(\theta) = \int_{-1}^{1} d(\cos\theta) \sum_{l'=0}^{\infty} (2l'+1)\, f_{l'}(k) P_l(\cos\theta) P_{l'}(\cos\theta)$$

with the use of formula $\int_{-1}^{1} d(\cos\theta) P_l(\cos\theta) P_{l'}(\cos\theta) = \frac{2}{2l+1}\delta_{l,l'}$.

Then, we get

$$I = \sum_{l=0}^{\infty} (2l'+1)\, f_{l'}(k) \frac{2}{2l+1}\delta_{l,l'} \quad = (2l+1) f_l(k) \frac{2}{2l+1} = 2f_l(k)$$

Thus, we have

$$\begin{aligned} f_l(k) &= \frac{1}{2}\int_{-1}^{1} d(\cos\theta) P_l(\cos\theta) f(\theta) \\ &= \frac{1}{2}\int_{-1}^{1} d(\cos\theta) P_l(\cos\theta) \left(-\frac{2mV_0}{\hbar^2\mu}\right) \frac{1}{2k^2(1-\cos\theta)+\mu^2} \\ &= -\frac{mV_0}{\mu\hbar^2k^2}\frac{1}{2}\int_{-1}^{1} dz \frac{P_l(z)}{1+\frac{\mu^2}{2k^2}-z} \\ &= -\frac{mV_0}{\mu\hbar^2k^2} Q_l\left(1+\frac{\mu^2}{2k^2}\right) \end{aligned}$$

where $Q_l(\varsigma)$ is the Legendre function of the second kind and is defined by

$$Q_l(x) = \frac{1}{2}\int_{-1}^{1} dz \frac{P_l(z)}{x-z}$$

with

$$x = 1 + \frac{\mu^2}{2k^2}.$$

We make a plot of $Q_l(x)$ as a function of x for $x > 1$, where l is changed as a parameter. (numerical integration is done by using the Mathematica).

(b) (i) As is shown in the above figure, we have $Q_l(x) > 0$ for $x > 1$.

$$x = 1 + \frac{\mu^2}{2k^2}$$

(ii) de Broglie wave length $\lambda = \frac{2\pi}{k} \gg \frac{1}{\mu}$ (the range of potential) or

$$\begin{aligned}
\frac{\mu}{k} &\gg 1 \\
f_l(k) &= -\frac{mV_0}{\mu\hbar^2k^2} Q_l\left(1 + \frac{\mu^2}{2k^2}\right) \\
&\approx -\frac{mV_0}{\mu\hbar^2k^2} Q_l\left(\frac{\mu^2}{2k^2}\right) \\
&= -\frac{mV_0}{\mu\hbar^2k^2} \frac{l!}{(2l+1)!!}\left(\frac{2k^2}{\mu^2}\right)^{l+1} \\
&= -\frac{mV_0}{\hbar^2\mu^{2l+3}} \frac{2^{l+1}l!}{(2l+1)!!} k^{2l+1}
\end{aligned}$$

or

$$f_l(k) = -\frac{mV_0}{\hbar^2\mu^2} \frac{2^{l+1}l!}{(2l+1)!!}\left(\frac{k}{\mu}\right)^{2l+1} = -\frac{\lambda}{8\pi} \frac{2^{l+1}l!}{(2l+1)!!}\left(\frac{k}{\mu}\right)^{2l+1}$$

11. The effective range: Phase shift (Capri)

The phase shift for $l = 0$ (s-wave) is given by 44

$$\begin{aligned}
\sin\delta_0 &= -\frac{2m}{\hbar^2} k \int_0^\infty dr r^2 V(r) \left[\frac{\sin(kr)}{kr}\right]^2 \\
&= -\frac{2m}{\hbar^2} k \int_0^\infty dr r^2 \frac{V_0 e^{-\mu}}{\mu r} \left[\frac{\sin(kr)}{kr}\right]^2 \\
&= -\frac{2m}{\hbar^2} \frac{kV_0}{\mu} \int_0^\infty dr^2 \frac{e^{-\mu}}{r} \left[\frac{\sin(kr)}{kr}\right]^2 \\
&= -\frac{\lambda}{16\pi} \frac{\mu}{k} \ln\left(1 + \frac{4k^2}{\mu^2}\right) \\
&= -\frac{\beta}{4} \frac{\mu}{k} \ln\left(1 + \frac{4k^2}{\mu^2}\right)
\end{aligned}$$

where

$$\lambda = 4\pi \frac{2mV_0}{\hbar^2\mu^2}, \quad \beta = \frac{2mV_0}{\hbar^2\mu^2} = \frac{\lambda}{4\pi}$$

and

$$\int_0^\pi dr r^2 \frac{e^{-\mu r}}{r} \left[\frac{\sin(kr)}{kr}\right]^2 = \frac{1}{4k^2} \ln\left(1 + \frac{4k^2}{\mu^2}\right)$$

Thus, we get

$$\begin{aligned}\sin\delta_0 &= -\frac{\beta}{4}\frac{\mu}{k}\ln\left(1+\frac{4k^2}{\mu^2}\right)\\ &= -\frac{\beta}{4}\frac{\mu}{k}\left(\frac{4k^2}{\mu^2}-\frac{8k^4}{\mu^4}\right)\\ &= -\beta\frac{k}{\mu}\left(1-\frac{2k^2}{\mu^2}\right)\end{aligned}$$

Note that

$$k\cot\delta_0 = k\frac{\cos\delta_0}{\sin\delta_0}$$

and

$$\cos\delta_0 = \sqrt{1-\sin^2\delta_0} = \sqrt{1-\frac{\beta^2k^2}{\mu^2}\left(1-\frac{2k^2}{\mu^2}\right)^2} \simeq \sqrt{1-\frac{\beta^2k^2}{\mu^2}} \approx 1-\frac{\beta^2k^2}{2\mu^2}$$

$$k\cot\delta_0 = k\frac{\cos\delta_0}{\sin\delta_0} = -k\frac{\beta^2k^2}{2\mu^2} \simeq -\frac{\mu}{\beta}\left(1-\frac{\beta^2k^2}{2\mu^2}\right)\left(1+\frac{2k^2}{\mu^2}\right) = -\frac{\mu}{\beta}+\frac{1}{2}k^2\left(\beta-\frac{4}{\beta}\right)\frac{1}{\mu} = -\frac{1}{a}+\frac{1}{2}r_0k^2$$

where a is the scattering length and r_0 is the effective range.

$$a = \frac{\beta}{\mu} = \frac{\lambda}{4\pi\mu}, r_0 = \frac{1}{\mu}\left(\beta-\frac{4}{\beta}\right)$$

Note that our result of r_0 is a little different from that reported by Capri. The parameter β is dimensionless. For the low energy limit, the condition for the Born approximation is $\lambda \ll 4\pi$,

leading to $a \ll \frac{1}{\mu}$. For the high energy limit, the condition for the Born approximation is $|\lambda| \ll 4\pi\frac{k}{\mu}$, leading to $a \ll \frac{1}{\mu}\frac{k}{\mu}$.

We note that the total cross section (the first order Born approximation) is given by

$$\sigma^{(1)} = \frac{\lambda^2}{4\pi}\frac{1}{\mu^2+4k^2}$$

In the limit of $k \to 0$, we have

$$\sigma^{(1)}(k=0) = \frac{1}{4\pi}\frac{\lambda^2}{\mu^2} = 4\pi a^2$$

using the scattering length a. Thus, the scattering length determines the low-energy scattering cross section. We see that

$$f_0(k) = S_0(k)-1 \quad = e^{2\delta_0(k)}-1 = \frac{2i}{\cot\delta_0(k)-1} \quad = \frac{2i\sin\delta_0(k)}{\cos\delta_0(k)-\sin\delta_0(k)} = \frac{2i\sin\delta_0(k)}{1-\sin\delta_0(k)} \quad = \frac{2ka}{i-ka}$$

where $\sin[\delta_0(k)] = -k\frac{\beta}{\mu} = -ka$. Thus, $f_0(k)$ has a single pole at $k = \frac{i}{a}$. This pole corresponds to a bound state of energy $E_b = -\frac{\hbar^2\kappa^2}{2m}$ and $\kappa = \frac{1}{a}$. Since the bound state is of the form $\exp(-\kappa r)/r$, its extension is a. ((Mathematica)) Calculation

$$\begin{aligned}&\text{g4} \;=\; \frac{1}{\mu}\frac{e^{-\mu r}}{k^2 r}\sin[kr]^2;\\ &\text{s1} \;=\; \text{Integrate}\,[g4,\{r,0,\infty\},\\ &\text{Assumptions}\;\to\{\mu>0,k>0\}]\\ &\left.\frac{\log\left[1+\frac{4k^2}{\mu^2}\right]}{4k^2\mu}\right|\end{aligned}$$

12. Optical theorem (Capri)

The scattering amplitude for low energy s-waves may be written as

$$\begin{aligned} f_0(k) &= \frac{e^{2i\delta_0}-1}{2ik} \\ &= \frac{1}{2ik}e^{i\delta_0}\left(e^{i\delta_0}-e^{-i\delta_0}\right) \\ &= \frac{1}{2ik}2i\sin\delta_0 e^{i\delta_0} \\ &= \frac{\sin\delta_0}{ke^{-i\delta_0}} \\ &= \frac{\sin\delta_0}{k\cos\delta_0 - ik\sin\delta_0} \\ &= \frac{1}{k\cot\delta_0 - ik} \end{aligned}$$

We note that

$$k\cot\delta_0 = -\frac{1}{a}+\frac{1}{2}r_0k^2,$$

where a is the scattering length and r_0 is the effective range. Thus, we get

$$\begin{aligned} f_0(k) &= \frac{1}{-\frac{1}{a}+\frac{1}{2}r_0k^2-ik} \\ &= -\frac{a}{1+iak-\frac{1}{2}r_0ak^2} \end{aligned}$$

The optical theorem states that the total cross-section σ is given by

$$\begin{aligned} \sigma &= \frac{4\pi}{k}\operatorname{Im}\left[f_0(k)\right] \\ &= \frac{4\pi}{k}\operatorname{Im}\left[\frac{\sin\delta_0}{ke^{-i\delta_0}}\right] \\ &= \frac{4\pi}{k}\frac{1}{k}\sin^2\delta_0 \end{aligned}$$

On the other hand, the total cross section is given by

$$\sigma = \int\frac{d\sigma}{d\Omega}d\Omega \quad = \int\left|f_0(k)\right|^2 d\Omega = 4\pi\left|f_0(k)\right|^2 \quad = 4\pi\left|\frac{\sin\delta_0}{ke^{-i\delta_0}}\right|^2 = \frac{4\pi}{k^2}\sin^2\delta_0$$

So, in this, the optical theorem is proved. We now use the expression of

$$f_0(k) = -\frac{a}{1+iak-\frac{1}{2}r_0ak^2}.$$

Thus, we have

$$\sigma = \frac{4\pi}{k}\operatorname{Im}\left[f_0(k)\right] \quad = \frac{4\pi}{k}\frac{a^2k}{\left(1-\frac{1}{2}r_0ak^2\right)^2+a^2k^2} = \frac{4\pi a^2}{\left(1-\frac{1}{2}r_0ak^2\right)^2+a^2k^2}$$

On the other hands by direct calculation, we find that

$$\sigma = \int\frac{d\sigma}{d\Omega}d\Omega \quad = \int\left|f_0(k)\right|^2 d\Omega = 4\pi\left|f_0(k)\right|^2 \quad = \frac{4\pi a^2}{\left(1-\frac{1}{2}r_0ak^2\right)^2+a^2k^2}$$

Thus, in this case, we also verify the optical theorem.

GKKG.13.13 2nd order scattering on e^{-r^2/R^2}

In the 2nd order of perturbation theory, find the scattering amplitude in the potential $U(r) = U_0e^{-r^2/R^2}$ for large momenta transferred, $qR \gg 1$. Compare the real and imaginary parts of $f^{(2)}$ with each other and with the Born amplitude.

Solution

The Fourier component of the potential is

$$\tilde{U}(q) = \int U_0 \exp\left\{-i\mathbf{q}\cdot\mathbf{r} - \frac{r^2}{R^2}\right\} dV = \pi^{3/2} U_0 R^3 e^{-q^2R^2/4}$$

and according to Eq. (2) from Problem 13.10, the scattering amplitude in the 2nd order of perturbation theory is described by the expression:

$$f^{(2)}(\mathbf{k},\mathbf{k}_0) = \frac{m^2}{8\pi^4\hbar^4}\int \frac{\tilde{U}(\mathbf{k}-\kappa)\tilde{U}(\boldsymbol{\kappa}-\mathbf{k}_0)}{\kappa^2 - k_0^2 - i\varepsilon} d^3\kappa = \frac{m^2U_0^2R^6}{8\pi\hbar^4} e^{-q^2R^2/4} \int \frac{\exp\left\{-\frac{1}{2}R^2\left[\kappa - \frac{1}{2}(\mathbf{k}+\mathbf{k}_0)\right]^2\right\}}{\kappa^2 - k_0^2 - i\varepsilon} d^3\kappa \tag{1}$$

The dominant role in the integral comes from the region of values $\boldsymbol{\kappa}$, where $|\boldsymbol{\kappa}$ - $(\mathbf{k}+\mathbf{k}_0)/2|R \leq 1$ (outside of this domain, the integrand is exponentially small). For large energies, $kR \gg 1$, and large momenta transfered, $qR \gg 1$, in this domain the denominator of the integrand in Eq. (1) changes only slightly, and it can be factored outside the integral sign at the point $\boldsymbol{\kappa} = \mathbf{k} + \mathbf{k}_0/2$. Then, a simple integration gives (for $k^2 = k_0^2$):

$$f^{(2)}(\mathbf{k},\mathbf{k}_0) \approx \mathrm{Re}\, f^{(2)} \approx -\frac{\sqrt{2\pi}m^2U_0^2R^3}{\hbar^4 q^2} \exp\left\{-\frac{1}{8}q^2R^2\right\} \tag{2}$$

In this approximation, amplitude $f^{(2)}$ is a real function. Its imaginary part according to Eq. (1) could be easily found in general if we note that

$$\mathrm{Im}\,\frac{1}{\kappa^2 - k_0^2 - i\varepsilon} = \pi\delta\left(\kappa^2 - k_0^2\right)$$

(compare to Problem 13.11). Writing $d^3\kappa = \kappa d\kappa^2 d\Omega/2$ and integrating first over κ^2 and then over the angles (choosing the polar axis along the vector $\mathbf{k}+\mathbf{k}_0$), we find:

$$\begin{aligned}\mathrm{Im}\, f^{(2)} &= \left(\frac{mU_0R^3}{4\hbar^2}\right)^2 \iint \kappa\delta\left(\kappa^2 - k^2\right) \exp\left\{-\kappa^2R^2 + \frac{1}{2}\boldsymbol{\kappa}\cdot(\mathbf{k}+\mathbf{k}_0)R^2\right\} d\kappa^2 d\Omega = \\ &= \frac{\pi m^2U_0^2R^4}{2\hbar^4|\mathbf{k}+\mathbf{k}_0|} \sinh\left(\frac{1}{2}|\mathbf{k}+\mathbf{k}_0|kR^2\right) e^{-k^2R^2}\end{aligned} \tag{3}$$

(Note that $|\mathbf{k}+\mathbf{k}_0| = \left(4k^2 - q^2\right)^{1/2}$.)
For large energies, $kR \gg 1$, and small scattering angles, when $qR \leq 1$, the scattering amplitude of the 2nd order is determined mainly by the imaginary part of Eq. (3), as is seen from Problem 13.14 (Eq. (2) for $qR \leq 1$ is not applicable). For large changes of momentum, on the contrary, the integral is dominated by the real part of the scattering amplitude, $f^{(2)}$. Moreover, since

$$\mathrm{Re}\, f^{(2)} \propto e^{-q^2R^2/8}, \text{ while } f^{(1)} = f^a \propto \tilde{U}(q) \propto e^{-q^2R^2/4}$$

then for the values of qR large enough, $\left|\mathrm{Re}\, f^{(2)}\right| \gg \left|f^B\right|$. This signal a break-down of the Born approximation, independently of the parameter U_0 that characterizes the interaction strength. [320] Let us emphasize that the discovered properties are characteristic for potentials with an exponential decrease of the Fourier component $\tilde{U}(q) \propto \exp\{-\alpha q^n\}$ with $n \geq 1$ for $q \to \infty$ (compare to Problem 8.29, and also to the case of a power-law decrease of $\tilde{U}(q)$, considered in the previous problem).
In conclusion, let us note that using Eq. (3) and the optical theorem (XIII.11), we can find the scattering cross-section in the Born approximation; the result, of course, coincides with its calculation by the equation $\sigma_B = \int \left(f^B\right)^2 d\Omega$ (see Problem 13.1 f).
[320] It corresponds to the large values of qR (the contribution of which to the total cross-section is small).

17.3.10 Problems about scattering in Born approximation 3

GKKG.13.14 Formula for 2nd order and low momenta transfered

Prove that the scattering amplitude of second-order perturbation theory for large energies, $kR \gg 1$, but for relatively low momenta transfered, $qR \lesssim 1$, is described by (R is the radius of the potential)

$$f^{(2)} \approx i\frac{m^2}{4\pi\hbar^4 k} \iint \left[\int_{-\infty}^{\infty} U(\boldsymbol{\rho}, z)dz\right]^2 \exp\{-i\mathbf{q}_\perp\cdot\boldsymbol{\rho}\}\, d^2\rho$$

Here $|\mathbf{q}_\perp| \approx q$, where $\mathbf{q}_\perp$ is the component of $\mathbf{q}$ perpendicular to the initial momentum $\mathbf{k}_0$ (directed along the axis z).

Apply this result to the potential $U(r) = U_0 e^{-r^2/R^2}$, and compare to Problem 13.13.

Solution

In the 2nd order of perturbation theory, the scattering amplitude is given by

$$f^{(2)}(\mathbf{k}, \mathbf{k}_0) = \frac{m^2}{8\pi^4\hbar^4} \int \frac{\tilde{U}(\mathbf{k}-\boldsymbol{\kappa})\tilde{U}(\boldsymbol{\kappa}-\mathbf{k}_0)}{\kappa^2 - k_0^2 - i\varepsilon} d^3\kappa \tag{1}$$

See Problem 13.10. For a large energy, $kR \gg 1$, and a small scattering angle, $qR \leq 1$, the vector $\boldsymbol{\kappa}$, as well as $\mathbf{k}$, is "close" to $\mathbf{k}_0$. Let us write these vectors in the form:

$$\mathbf{k} = \mathbf{k}_0 + \mathbf{q} = k_\parallel \mathbf{n}_0 + \mathbf{q}_\perp, \quad \kappa = \kappa_\parallel \mathbf{n}_0 + \boldsymbol{\kappa}_\perp$$

where $\mathbf{n}_0 = \mathbf{k}_0/k_0$, while $\mathbf{q}_\perp, \boldsymbol{\kappa}_\perp \perp \mathbf{n}_0$. See that $|\mathbf{q}_\perp| \approx q$ and $k_\parallel = k_0 + q_\parallel, q_\parallel \approx -q^2/2k_0$. Compare to Problem 13.2. After substitution of the explicit expression for Fourier components of the potential (in terms of $U(\mathbf{r})$), the integral in Eq. (1) takes the form:

$$\int \frac{U(\boldsymbol{\rho}_1, z_1) U(\boldsymbol{\rho}_2, z_2) \exp\left\{-i\left[\kappa'_\parallel (z_1 - z_2) + \boldsymbol{\kappa}_\perp \cdot (\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2) + \mathbf{q}_\perp \cdot \boldsymbol{\rho}_2\right]\right\}}{2k_0\kappa'_\parallel + \left(\kappa'_\parallel\right)^2 + \kappa_\perp^2 - i\varepsilon} d^3r_1 d^3r_2 d\kappa'_\parallel d^2\kappa_\perp \tag{2}$$

Here $\boldsymbol{\kappa}'_\parallel = \boldsymbol{\kappa}_\parallel - \mathbf{k}_0$, and the term $-iq_\parallel z_2$ in the exponent is omitted, since $\left|q_\parallel z_2\right| \leq q^2 R/k_0 \ll 1$. Let us note that the terms in the perturbative expansion for the scattering amplitude (see Eq. (2) from Problem 13.10) could be interpreted as describing a number of single-particle collisions with the scattering potential, each accompanied by a momentum change for the particle being scattered. In this sense, the radiusvector $\mathbf{r}_1$ in the corresponding integral corresponds to the point of first collision, after which the particle momentum becomes equal to $\boldsymbol{\kappa}$ (after the second collision, it takes the value $\mathbf{k}$).

Closing the contour in the upper half-plane of the complex variable $\kappa'_\parallel$ in the case of $z_2 > z_1$, and in the lower half-plane for $z_2 < z_1$, we can perform the integration over $\kappa'_\parallel$ in Eq. (2) :

$$\int \frac{\exp\left\{-i\kappa'_\parallel (z_1 - z_2)\right\} d\kappa'_\parallel}{2k_0\kappa'_\parallel + \left(\kappa'_\parallel\right)^2 + \kappa_\perp^2 - i\varepsilon} = \begin{cases} \frac{i\pi}{k_0} \exp\left\{\frac{i\kappa_\perp^2}{2k_0}(z_1 - z_2)\right\}, z_2 > z_1 \\ \frac{i\pi}{k_0} \exp\left\{2ik_0 (z_1 - z_2)\right\}, z_2 < z_1 \end{cases} \tag{3}$$

If $|k_0 z_{1,2}| \sim k_0 R \gg 1$, then in the case of $z_1 > z_2$, the exponent in Eq. (3) is a fast oscillating function. This means that for the subsequent integration over $z_{1,2}$ in Eq. (2),
a contribution of such $z_{1,2}$ would be small, and can be neglected. Thus, Eq. (3) could be considered equal to

$$\frac{i\pi}{k_0} \eta(z_2 - z_1) \exp\left\{i \frac{\kappa_\perp^2 (z_1 - z_2)}{2k_0}\right\} \tag{4}$$

where $\eta(z)$ is a step function, [322] and since typically we have $z_{1,2} \lesssim R$ and $\kappa_\perp \lesssim R^{-1}$, then the exponent can be replaced by 1. The appearance of a step function in Eq. (4) has a physical explanation: for fast particles, each successive "collision" takes place for larger and larger values of z (there is no backward scattering).

Now, in Eq. (2), integration over $\boldsymbol{\kappa}_\perp$ is easily performed, and the δ-function, $\delta(\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2)$, allows integration over $\boldsymbol{\rho}_2$. As a result, we obtain

$$f^{(2)} = i \frac{m^2}{2\pi\hbar^4 k_0} \int \left\{ \int_{-\infty}^{\infty} U(\boldsymbol{\rho}, z_1) dz_1 \int_{z_1}^{\infty} U(\boldsymbol{\rho}, z_2) dz_2 \right\} e^{-i\mathbf{q}_\perp \cdot \boldsymbol{\rho}} d^2\rho$$

Finally, replacing the lower limit of integration over z_2 by $-\infty$ and introducing the coefficient $1/2$, we obtain the expression given in the problem condition. Let us note that for a central potential, the scattering amplitude is purely imaginary (a real part of the amplitude $f^{(2)}$ is much smaller than the imaginary part, and in this approximation it does not appear; compare to Problems 13.12 and 13.13).

For the potential $U = U_0 \exp\left\{-r^2/R^2\right\}$, we obtain

$$f^{(2)} = i \frac{\pi m^2 U_0^2 R^4}{8\hbar^4 k_0} e^{-q^2 R^2/8}$$

which coincides with Eq. (3) from Problem 13.13 for the values $qR \lesssim 1$.

In conclusion, note that taking $q = 0$ in the equation for $f^{(2)}$ and using the optical theorem (XIII.11), we obtain the scattering cross-section in the Born approximation, which coincides with the result of Problem 13.2.

GKKG.13.15 Lippmann-Schwinger equation for special case

From the solution of the Lippmann-Schwinger equation (see Problem 13.10), find the scattering amplitude for a separable potential with the following integral kernel $U(r, r') = \lambda\chi(r)\chi^*(r')$. Find the angular distribution and total scattering cross-section.

Solution

(??? из условия не понятно, что за ядро потенциала?? пока думаю, что это просто такой потенциал, а слова лишние тут. мб изменю потом условие.)

The Lippmann-Schwinger equation (Eq. (1) from Problem 13.10) remains valid for an arbitrary interaction $\hat{U}$, if we replace the potential Fourier component $\tilde{U}(\mathbf{k} - \mathbf{k}')$ by the corresponding kernel $\tilde{U}(\mathbf{k}, \mathbf{k}')$. For the separable potential,

$$\tilde{U}(\mathbf{k}, \mathbf{k}') = \lambda g(k) g^*(k'), \quad g(k) = \int e^{-i\mathbf{k}\cdot\mathbf{r}}\chi(r)dV$$

and the Lippmann-Schwinger equation reads

$$f(\mathbf{k}, \mathbf{k}_0) = -\frac{\lambda m}{2\pi\hbar^2} g(k)\left[g^*(k_0) + \int \frac{g^*(\kappa) f(\mathbf{k}, \mathbf{k}_0)\, d^3\kappa}{2\pi^2(\kappa^2 - k_0^2 - i\varepsilon)}\right] \tag{1}$$

Denoting the integral here by $F(k_0)$, we have

$$f(\mathbf{k}, \mathbf{k}_0) = -\frac{\lambda m}{2\pi\hbar^2} g(k)\left[g^*(k_0) + F(k_0)\right]$$

and after substituting this expression back into the integral, we obtain a self-consistent equation for $F(k_0)$ and determine the scattering amplitude ($k = k_0$):

$$f(\mathbf{k}, \mathbf{k}_0) \equiv f(k) = -\frac{\lambda m}{2\pi\hbar^2}\frac{g^2(k)}{1 + K(k)}$$

where

$$K(k) = \frac{\lambda m}{4\pi^3\hbar^2}\int \frac{|q(\kappa)|^2 d^3\kappa}{\kappa^2 - k^2 - i\varepsilon}$$

One of the notable properties of the scattering amplitude is its independence from the scattering angle, [323] so that the angular distribution of the scattered particles is isotropic, and the total scattering cross-section is simply $\sigma(E) = 4\pi|f|^2$ (it is informative to prove its consistence with the optical theorem). Note that in the largeenergy limit: $\sigma(E) \propto |g(k)|^4$ for $E \to \infty$.

GKKG.13.16 Difference between repulsive potential and an attractive without bound states

For $E = 0$, compare the values of the exact and Born scattering amplitudes in a potential $U(r)$ for
a) a repulsive potential $U(r) \geq 0$;
b) an attractive potential in which there are no bound states (i.e., the potential well is "shallow" enough).

Prove that the Born approximation in case a) overestimates the scattering cross-section, while in case b), it underestimates it.

Solution

For $E = 0$, we have

$$f^B(0) = -\frac{m}{2\pi\hbar^2}\int U(r)dV, \quad f_{ex}(0) = -\frac{m}{2\pi\hbar^2}\int U(r)\psi_0(r)dV \tag{1}$$

where the wavefunction $\psi_0(r)$ satisfies the equation:

$$\psi_0(r) = 1 - \frac{m}{2\pi\hbar^2}\int U(r')\frac{1}{|\mathbf{r} - \mathbf{r}'|}\psi_0(r')\, dV' \tag{2}$$

If there are no bound states in the potential $U(r)$, then the wavefunction for $E = 0$ has no zeros, and since $\psi_0(\infty) = 1$, then $\psi_0(r) > 0$. As follows from Eq. (2), for a repulsive potential, $0 \leq \psi_0(r) \leq 1$, and according to Eq. (1), we have the inequality $\left|f^B(0)\right| > |f_{\text{ex}}(0)|$, i.e., the Born approximation overestimates the

scattering cross-section. In the analogous case of an attractive potential, $U(r) \leq 0$, we obtain $\left|f^B(0)\right| < |f_{ex}(0)|$, so the Born approximation underestimates the scattering cross-section (in the absence of bound states in the potential). Let us emphasize that the relations between the cross-sections do not assume that the potential is weak, as required for the Born approximation to be formally valid. In connection to this problem, see also Problems 13.69 and 13.70.

GKKG.13.17 Scattering by a magnetic field

In the Born approximation, obtain a scattering amplitude for scattering of a charged particle by a magnetic field, $\mathcal{H}(\mathbf{r})$. Prove gauge invariance of the result obtained.

Solution

To first order in the magnetic field, the interaction has the form:

$$\hat{V} = -\frac{e}{2mc}(\hat{\mathbf{p}} \cdot \mathbf{A} + \mathbf{A} \cdot \hat{\mathbf{p}})$$

Substituting this expression into Eq. (XIII.5) instead of $U(r)$, and replacing the wavefunction $\psi^+_{\mathbf{k}_0}$ by a plane wave, we obtain the scattering amplitude

$$f(\mathbf{k}, \mathbf{k}_0) = \frac{e}{4\pi\hbar^2 c}\int e^{-i\mathbf{k}\cdot\mathbf{r}}(\hat{\mathbf{p}} \cdot \mathbf{A} + \mathbf{A} \cdot \hat{\mathbf{p}})e^{i\mathbf{k}_0\cdot\mathbf{r}}d^3r = \frac{e}{4\pi\hbar c}(\mathbf{k} + \mathbf{k}_0) \cdot \tilde{\mathbf{A}}(\mathbf{q})$$

where $\tilde{\mathbf{A}}(\mathbf{q}) = \int e^{-i\mathbf{q}\cdot\mathbf{r}}\mathbf{A}(\mathbf{r})dV$ is the Fourier transform of the vector potential. Under a gauge transformation, a term $\boldsymbol{\nabla}\chi(\mathbf{r})$ is added to $\mathbf{A}(\mathbf{r})$, and consequently $i\mathbf{q}\tilde{\chi}(\mathbf{q})$ to $\tilde{\mathbf{A}}(\mathbf{q})$. But since $\mathbf{q} \cdot (\mathbf{k} + \mathbf{k}_0) = 0$, then the value of f and the value of the differential scattering cross-section do not change, in accordance with gauge invariance.

me. Scattering in 2D in 2nd order of Born approximation (???)

Using the 2nd order of Born approximation, find the scattering amplitude for the two-dimensional space and the total scattering cross-section of a particle on the following potentials:
a) $U(r) = \frac{\alpha}{r}e^{-r/R}$
b) $U(r) = \alpha\delta(r - R)$;
c) $U(r) = U_0 e^{-r/R}$

Solution.

(такое пока что не продумывал. идея взять любой шаблонный и попробовать решить. формулы все есть, потом попробую)

17.3.11 Problems about partial-wave analysis 1

В этом разделе задачи, которые важно прорешать для понимания рассеяния.

Б-2.12.8 Эффект Рамзауэра (!!!!)

Найти сечение рассеяния медленных частиц на сферически-симметричной прямоугольной потенциальной яме. Определить, при каких соотношениях между глубиной V_0 и радиусом ямы a полное сечение намного превышает геометрическое значение πa^2 (резонансное рассеяние) и, наоборот, обращается в ноль (эффект Рамзауэра).
Дополнительный вопрос: а что происходит с быстрыми частицами?

Solution. по Киселеву

(это нужно хорошо продумать!!!)

Потенциал ямы есть $U(r) = \begin{cases} -U_0, & r < a_0 \\ 0, & r > a_0 \end{cases}$

Решение уравнения Шредингера для радиальной волновой функции при $l = 0$ запишется в общем виде как

$$R_{k0}(r) = \begin{cases} A\frac{\sin(k_u r)}{k_u r}, & k_u^2 = \frac{2m(E+U_0)}{\hbar^2}, \quad r < a_0 \\ B\frac{\sin(kr+\delta_0)}{kr}, & k^2 = \frac{2mE}{\hbar^2}, \quad r > a_0 \end{cases}$$

где A, B - константы, которые можно определить исходя из условия непрерывности волновой функции.

$$\left.\frac{R'_{k0}(r)}{R_{k0}(r)}\right|_{r=a_0-0} = \left.\frac{R'_{k0}(r)}{R_{k0}(r)}\right|_{r=a_0+0},$$

для медленных частиц $ka_0 \ll 1$ дифференцирование при $r = a_0 + 0$ дает

$$R'_{k0}(r) \sim k\frac{\cos(\bullet)}{kr} - \frac{\sin(\bullet)}{kr^2} = \frac{1}{kr^2}\{kr\cos(\bullet) - \sin(\bullet)\}$$

а при $r = a_0 - 0$ в глубокой яме $k_u a_0 \gg 1$

$$R'_{k0}(r) \sim k_u\frac{\cos(*)}{k_u r} - \frac{\sin(*)}{k_u r^2} = \frac{1}{k_u r^2}\{k_u r\cos(*) - \sin(*)\}$$

Подставляя, получаем $\tan(ka_0 + \delta_0) = \frac{k}{k_u}\tan(k_u a_0)$, откуда

$$\delta_0 = -ka_0 + \arctan\left[\frac{k}{k_u}\tan(k_u a_0)\right]$$

Если $\tan(k_u a_0) \to \pm\infty$, то вкладом $ka_0 \to 0$ следует пренебречь и $\delta_0 \to \pm\pi/2$, так что имеет место резонанс: сечение рассеяния принимает максимально допустимое значение для парциальной волны $l = 0$, и оно существенно больше геометрического значения $\sigma_0 = 4\pi/k^2 = 4\pi a_0^2/(ka_0)^2 \gg 4\pi a_0^2$ $k \to 0$ в яме $k_u \to k_u^0 = \sqrt{2mU_0}/\hbar$, и фаза

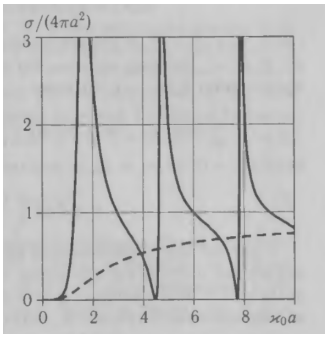
$$\delta_0 \approx k\left\{\frac{1}{k_u^0}\tan\left(k_u^0 a_0\right) - a_0\right\} = \frac{k}{k_u^0}\left\{\tan\left(k_u^0 a_0\right) - k_u^0 a_0\right\}$$

При условии

$$\tan\left(k_u^0 a_0\right) = k_u^0 a_0$$

фаза δ_0, а значит, и длина рассеяния обращаются в нуль, т.е. имеет место эффект Рамзауера: сечение рассеяния определяется высшими парциальными волнами, так что оно аномально мало, зависит от энергии и от углов.

При этом (13.44) совпадает с условием появления в яме связанного состояния.



Описание прохождения быстрых частиц ($ka \gg 1$).

Как мы уже выяснили, для быстрых частиц вклад в полное сечение дают парциальные волны с

$$l \leqslant ka \gg 1$$

При этом, поскольку максимальное значение парциального сечения $\sigma_l^{\max} = 4\pi(2l+1)/k^2$ Достигается при $\sin\delta_l = 1$, полное сечение не превышает величину

$$\sigma < \frac{4\pi}{k^2}\sum_{l=0}^{ka}(2l+1) = \frac{4\pi}{k^2}(ka+1)^2 \approx 4\pi a^2 = \sigma_{\text{geom}}$$

Б-2.12.9 Типичное рассеяние (???)

Найти сечение рассеяния медленных частиц на сферически-симметричном прямоугольном потенциальном барьере.

Solution.

(????!!!!)

Б-2.12.10 Сечение на непроницаемой сфере

Найти сечение рассеяния частиц на непроницаемой сфере радиуса a. Отдельно рассмотреть предельные случаи:
а) медленных частиц ($ka \ll 1$);
б) быстрых частиц ($ka \gg 1$).
Обсудить характер зависимости от угла θ дифференциальных сечений упругого рассеяния.

Solution. по Белоусову

К.? Сечение на непроницаемой сфере по Киселеву

Вклад частиц с $l \gg ka$ в сечение рассеяния пренебрежимо мал.
Для частиц с $l \leqslant ka$, определяющих сечение, радиальные волновые функции при $r > a$ мало отличаются от своих асимптотических выражений, справедливых при $kr \gg l$,

$$R_{kl}(r) \simeq A_l \frac{\sin\left(kr - \frac{\pi}{2}l + \delta_l\right)}{kr}, \quad k^2 = \frac{2mE}{\hbar^2}$$

По непрерывности волновой функции

$$R_{kl}(r)|_{r=a} = 0 \to \sin\left(ka - \frac{\pi}{2}l + \delta_l\right) \approx 0$$

откуда

$$\delta_l \approx -ka + \frac{\pi}{2}l$$

Для вклада парциальной волны

$$\sin^2\delta_l = \frac{1}{2}\left(1 - \cos 2\delta_l\right) = \frac{1}{2}\left\{1 - (-1)^l \cos 2ka\right\}$$

Поэтому в полном сечении

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{ka\gg 1}(2l+1)\sin^2\delta_l$$

можно выделить два вклада: первый дает

$$\frac{2\pi}{k^2}\sum_{l=0}^{ka\gg 1}(2l+1) = 2\pi a^2$$

а второй $-\frac{2\pi}{k^2}\cos(2ka)\sum\limits_{l=0}^{ka\gg 1}(2l+1)(-1)^l$ можно легко оценить согласно разбиению на четные и нечетные l:

$$\sum_{l=0}^{ka\gg 1}(2l+1)(-1)^l = \sum_{n=0}^{\frac{1}{2}ka\gg 1}(4n+1) - \sum_{n=0}^{\frac{1}{2}ka\gg 1}(4n+3) \approx n(2n+1) - n(2n+3)|_{n=\frac{1}{2}ka\gg 1}$$

и

$$-\frac{2\pi}{k^2}\cos(2ka)\sum_{l=0}^{ka\gg 1}(2l+1)(-1)^l \approx 2\pi a^2\frac{\cos(2ka)}{ka}, \quad |\frac{\cos(2ka)}{ka}| \ll 1$$

а значит, этот вклад подавлен по сравнению с первым, и им можно пренебречь.
В итоге, сечение определяется геометрической величиной

$$\sigma \approx 2\pi a^2$$

Б-2.12.11 Сечение рассеяния быстрых частиц на черном шаре

Найти полное сечение рассеяния быстрых частиц ($ka \gg 1$) на черном шаре радиуса a.

Solution.

(??? начало добавлю!)

Падающие на него волны, т.е. оно не отражает волны, достигшие его поверхности.

Как мы видели, центробежные силы создают потенциальный барьер, который непроницаем для волн с $l \gg k$ a.

Поэтому для этих волн отражение происходит также, как и в свободном случае: $S_l = 1$. При $l \leqslant ka$ волны достигают поверхности черного шара, и отражения не прои сходит: $S_l = 0$, а значит, имеет место неупругое рассеяние ($|S_l| < 1$). В этом случае сечение упругого рассеяния

$$\sigma_{\text{el}} = \frac{\pi}{k^2}\sum_{l=0}^{ka}(2l+1)|S_l - 1|^2 = \frac{\pi}{k^2}\sum_{l=0}^{ka}(2l+1) = \pi a^2$$

а неупругого

$$\sigma_{\text{inel.}} = \frac{\pi}{k^2}\sum_{l=0}^{ka}(2l+1)\left(1 - |S_l|^2\right) = \frac{\pi}{k^2}\sum_{l=0}^{ka}(2l+1) = \pi a^2 = \sigma_{\text{el.}}$$

Итак, упругое и неупругое сечения равны друг другу.

Найдем мнимую часть упругого рассеяния в перед

$$\text{Im}\mathfrak{m} f_l(0) = \text{Im}\mathfrak{m}\left[\frac{2l+1}{2\text{i}k}\left(S_l - 1\right)\right] = \frac{2l+1}{2k}$$

В итоге, Для каждого парциального сечения устанавливаем равенство

$$\sigma_l = \sigma_{\text{el}}^l + \sigma_{\text{inel.}}^l = \frac{4\pi}{k}\text{Im}\mathfrak{m} f_l(0) = \frac{2\pi}{k^2}(2l+1)$$

т.е. соотношение оптической теоремы для заданного типа рассеяния.

Б-2.12.12 Рассеяния α-частиц протонов друг на друге

Найти дифференциальное сечение рассеяния:
а) α-частиц на α-частицах;
б) протонов на протонах.

Общий подход к описанию рассеяния

(тут укажу суть решения, пока не вижу его четко. нужно переписать задачу, по сути мы свойства этого решения находим, а не саму величину!)

Волновая функция, описывающая движение двух тождественных частиц в системе центра масс, имеет вид

$$\Psi\left(\mathbf{r}_1, \mathbf{r}_2, s_1, s_2\right) = \Phi(\mathbf{R})\psi(\mathbf{r})\chi\left(s_1, s_2\right).$$

Здесь $\mathbf{R} = \frac{1}{2}\left(\mathbf{r}_1 + \mathbf{r}_2\right)$ - координата центра масс, функция $\Phi(\mathbf{R})$ описывает движение центра масс системы; $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ - относительная координата, функция $\psi(\mathbf{r})$ описывает движение частицы с приведенной массой $\mu = m/2$; $\chi\left(s_1, s_2\right)$ - спиновая функция двух частиц. Мы предположили, что потенциал взаимодействия не зависит от спинов, поэтому спиновые и координатные переменные разделяются.

Согласно постулату тождественности полная волновая функция Ψ должна быть симметричной или антисимметричной относительно перестановки частиц $1 \leftrightarrow 2$. Координата $\mathbf{R}$ не меняется при указанной перестановке, поэтому симметризации или антисимметризации подлежит только произведение $\psi(\boldsymbol{r})\chi\left(s_1, s_2\right)$.

а) α-частицы.

Спин α-частиц равен нулю, поэтому полная волновая функция должна быть симметричной относительно перестановки $1 \leftrightarrow 2$. При такой перестановке относительная координата меняет знак: $\mathbf{r} \to -\mathbf{r}$, и в сферической системе координат это эквивалентно замене $\theta \to \pi - \theta, \varphi \to \varphi + \pi, r \to r$. В соответствии со сказанным вид функции $\psi(\mathbf{r})$ при больших значениях r должен быть следующим:

$$\psi_s(\mathbf{r})|_{r\to\infty} \sim e^{i\mathbf{kr}} + e^{-i\mathbf{kr}} + (f(\theta) + f(\pi - \theta))\frac{e^{ikr}}{r}.$$

Здесь два первых слагаемых описывают начальное движение частиц в системе центра масс. Первое слагаемое описывает начальное состояние частицы с приведенной массой μ, налетающей на рассеивающий центр из $-\infty$. Второе же слагаемое описывает состояние такой же частицы, летящей из $+\infty$. Третье и четвертое слагаемые учитывают две возможности по рассеянию частицы с массой μ в поле рассеивающего центра. Частица, летящая из $-\infty$, может испытать рассеяние на угол θ и будет зарегистрирована там детектором, ее вероятность так рассеяться отражена в амплитуде $f(\theta)$. В этой же точке вероятность рассеяться второй частице равная определяется $f_2(\pi - \theta)$, ведь она рассеется $\pi - \theta$, и в силу тождественности частиц $f_2(\pi - \theta) = f(\pi - \theta)$.

Дифференциальное сечение рассеяния по определению это отношение числа частиц, рассеявшихся в единицу времени в элемент телесного угла $d\Omega$ в направлении детектора, к плотности потока в каждой из падающих волн, или:

$$d\sigma = |f(\theta) + f(\pi - \theta)|^2 d\Omega$$

б) Протоны.

Так как у протонов спин полуцелый, то полная волновая функция должна быть антисимметричной относительно перестановки частиц. В качестве спиновых функций будут выступать функции $\chi(S, M)$, собственные для операторов квадрата суммарного спина $\hat{\mathbf{S}}^2$ и проекции суммарного спина $\hat{\mathrm{S}}_2$.

(тут укажу решение этой задачи, см. 2.10.1)

Известно, что в состоянии с суммарным спином $S = 0$ спиновая функции антисимметрична, значит координатная функция должна быть симметричной, т. е. она должна быть равна сумме двух начальных вол и двух рассеянных с одинаковыми амплитудами рассеяния:

$$\psi_s(\mathbf{r})|_{r\to\infty} \sim e^{i\mathbf{kr}} + e^{-i\mathbf{kr}} + (f(\theta) + f(\pi - \theta))\frac{e^{ikr}}{r}.$$

В состояниях с $S = 1$ спиновые функции симметричные, поэтому функция $\psi(\mathbf{r})$ должна быть антисимметризована. Подводя итог, можно сказать, что в состояниях с полным спином протонов, равным S, дифференциальное сечение рассеяния равно

$$d\sigma_S = |f(\theta) + (-1)^S f(\pi - \theta)|^2 d\Omega.$$

Если же пучки исходных частиц неполяризованы, то будет наблюдаться среднее значение эффективного сечения. Считая, что все спиновые состояния равновероятны, получим

$$d\sigma = \frac{1}{4} d\sigma_{S=0} + \frac{3}{4} d\sigma_{S=1}.$$

ПТФ-14.з1;LL3-123.1 Фазовая теория в 2D

Постройте фазовую теорию рассеяния в двумерии для случая осесимметричных потенциалов. А именно, выразите через фазовые сдвиги δ_m амплитуду рассеяния $f(\varphi)$, парциальные сечения рассеяния σ_m и полное сечение σ, и выведите оптическую теорему.

Напоминание:

$$\psi_{2D}(\mathbf{r}) = e^{ikr\cos\varphi} + f_{2D}(\varphi)e^{i\frac{\pi}{4}}\frac{e^{ikr}}{\sqrt{r}}$$

Solution.

$$-\frac{\hbar^2}{2M}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2}\right) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

$$e^{ikz} \equiv e^{ikr\cos\varphi} = \sum_{m=-\infty}^{\infty} Q_m^{\text{free}}(r)e^{im\varphi}, \qquad Q_m^{\text{free}}(r) = \frac{1}{2\pi}\int_0^{2\pi} \exp(i(kr\cos\varphi - m\varphi))d\varphi \equiv i^m J_m(kr)$$

(??? откуда такая формула - не знаю, нужно умф дописывать! Однако, можно сослаться на ЛЛ3, там она написана.)

We consider for $r \gg 1$ that $kr \gg 1$, even if k is small,

$$Q_m^{\text{free}}(r; r \gg 1) \approx i^m \sqrt{\frac{2}{\pi kr}} \sin\left(kr - \frac{\pi}{2}\left(m - \frac{1}{2}\right)\right)$$

For $V \neq 0$

$$Q_m(r) \approx i^m \sqrt{\frac{2}{\pi kr}} \sin\left(kr - \frac{\pi}{2}\left(m - \frac{1}{2}\right) + \delta_m\right), \quad \delta_m = \delta_{-m}$$

$$\psi = \sum_{m=-\infty}^{\infty} C_m Q_m(r) e^{im\varphi}, \qquad f(\varphi) = \sum_{m=-\infty}^{\infty} f_m(\varphi) e^{im\varphi}$$

$$C_m Q_m(r) = Q_m^{\text{free}}(r) + f_m(\varphi) e^{i\frac{\pi}{4}} \frac{e^{ikr}}{r}$$

$$C_m \sqrt{\frac{2}{\pi kr}} \sin\left(kr - \frac{\pi}{2}\left(m - \frac{1}{2}\right) + \delta_m\right) = i^m \sqrt{\frac{2}{\pi kr}} \sin\left(kr - \frac{\pi}{2}\left(m - \frac{1}{2}\right)\right) + f_m(\varphi) e^{i\frac{\pi}{4}} \frac{e^{ikr}}{r}$$

$$\frac{C_m}{i} \sqrt{\frac{1}{2\pi kr}} \left(\exp\left(ikr - \frac{i\pi}{2}\left(m - \frac{1}{2}\right) + i\delta_m\right) - \exp\left(-ikr + \frac{i\pi}{2}\left(m - \frac{1}{2}\right) - i\delta_m\right)\right) =$$
$$= i^{m-1} \sqrt{\frac{1}{2\pi kr}} \left(\exp\left(ikr - \frac{i\pi}{2}\left(m - \frac{1}{2}\right)\right) - \exp\left(-ikr + \frac{i\pi}{2}\left(m - \frac{1}{2}\right)\right)\right) + f_m(\varphi) e^{i\frac{\pi}{4}} \frac{e^{ikr}}{\sqrt{r}}$$

$$\begin{cases} e^{-ikr} \\ e^{ikr} \end{cases} \Rightarrow C_m = e^{i\delta_m} i^m \qquad \Rightarrow \qquad \begin{cases} C_m = e^{i\delta_m} i^m, \\ i^{m-1} \sqrt{\frac{1}{2\pi kr}} \exp\left(-\frac{i\pi}{2}\left(m - \frac{1}{2}\right)\right)\left(e^{2i\delta_m} - 1\right) = f_m(\varphi) \frac{e^{i\frac{\pi}{4}}}{\sqrt{r}} \end{cases}$$

$$f_m(\varphi) = \frac{1}{i\sqrt{2\pi k}} (e^{2i\delta_m} - 1)$$

$$f(\varphi) = \sum_{m=-\infty}^{\infty} f_m(\varphi) e^{im\varphi} = \frac{1}{i\sqrt{2\pi k}} \sum_{m=-\infty}^{\infty} (e^{2i\delta_m} - 1) e^{im\varphi}.$$

$$\sigma = \int_0^{2\pi} |f(\varphi)|^2 d\varphi = \frac{1}{2\pi k} \sum_{m=-\infty}^{\infty} 4 \sin^2 \delta_m \cdot 2\pi = \frac{4}{k} \sum_{m=-\infty}^{\infty} \sin^2 \delta_m; \qquad \sigma_m = \frac{4}{k} \sin^2 \delta_m.$$

Here $\int\limits_0^{2\pi} d\varphi e^{i(m_2 - m_2)\varphi} = 0$ since $(m_2 - m_2) \in \mathbb{Z}$.

$$\text{Im} f(0) = \text{Im} \frac{1}{i\sqrt{2\pi k}} \sum_{m=-\infty}^{\infty} (e^{2i\delta_m} - 1) = \text{Im} \frac{1}{i\sqrt{2\pi k}} \sum_{m=-\infty}^{\infty} (\cos(2\delta_m) + i \sin(2\delta_m) - 1) =$$
$$= \frac{1}{\sqrt{2\pi k}} \sum_{m=-\infty}^{\infty} (1 - \cos 2\delta_m) = \sqrt{\frac{2}{\pi k}} \sum_{m=-\infty}^{\infty} \sin^2 \delta_m$$

$$\text{Im} f_{2D}(0) = \sqrt{\frac{k}{8\pi}} \sigma \qquad \text{(optic th 2d)}$$

ПТФ-14.з2. Потенциал $1/r^2$ в 2D

Найдите фазовые сдвиги и сечение рассеяния для двумерного потенциала $V(r) = \frac{\hbar^2 \beta}{2mr^2}$. Исследуйте предел слабого ($\beta \ll 1$, с точностью до членов $O(\beta^2)$) и сильного ($\beta \gg 1$) потенциала.

Reminder:

$$\sigma_{m\ 2D} = \frac{4}{k} \sin^2 \delta_m \qquad \text{Im} f_{2D}(0) = \sqrt{\frac{k}{8\pi}} \sigma$$

Solution.

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + \frac{\hbar^2\beta}{2mr^2} = -\frac{\hbar^2}{2m}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right) + \frac{\hbar^2\beta}{2mr^2}$$

$$\psi(\mathbf{r}) \equiv \sum_{l=-\infty}^{\infty} q_l(r)e^{il\varphi}$$

$$\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

$$-\frac{\hbar^2}{2m}\left(q_l''(r) + \frac{q_l'(r)}{r} - \frac{l^2}{r^2}q_l(r)\right) + \frac{\beta\hbar^2 q_l(r)}{2mr^2} = Eq_l(r)$$

$$r^2q_l''(r) + rq_l'(r) + \left(\frac{2mEr^2}{\hbar^2} - l^2 - \beta\right)q_l(r) = 0.$$

$z \equiv \frac{\sqrt{2mE}}{\hbar}r$,

$$z^2q_l''(z) + zq_l'(z) + \left(z^2 - l^2 - \beta\right)q_l(z) = 0 \qquad \text{(Bessel eq.)}$$

$$q_l(z) = J_{\sqrt{l^2+\beta}}(z) \approx \sqrt{\frac{2}{\pi z}}\cos\left(z - \frac{\pi}{2}\sqrt{l^2+\beta} - \frac{\pi}{4}\right)$$

We also know that $Q_m(r) \approx i^m\sqrt{\frac{2}{\pi kr}}\sin\left(kr - \frac{\pi}{2}\left(m - \frac{1}{2}\right) + \delta_m\right); \delta_m = \delta_{-m}$

Мы воспользовались $\sin(x + \pi/2) = \cos(x)$. (??? я так и не понял, что делать с i^m? Если почему-то просто проигнорировать, то у меня получается еще дополнительный (-π), что на ответ не влияет, потому что будем в квадрат синус возводить. Вопрос - что с i делать-то? Модуль - обобщает формулу с учетом $\delta_m = \delta_{-m}$. тоже непонятно, как получить ее, без обобщения, а просто для отрицательных m)

$$\delta_l = \frac{\pi}{2}\left(|l| - \sqrt{l^2+\beta}\right)$$

$$\sigma = \frac{4}{k}\sum_{l=-\infty}^{\infty}\sin^2\left(\frac{\pi}{2}(|l| - \sqrt{l^2+\beta})\right)$$

For $\beta \ll 1 \Rightarrow$ for $l \neq 0$ $\delta_l = \frac{\pi}{2}\left(|l| - |l|\sqrt{1+\frac{\beta}{l^2}}\right) \approx -\frac{\pi\beta}{4|l|}$,

$$\begin{cases}\delta_l = -\frac{\pi\beta}{4|l|}, & l \neq 0\\ \delta_0 = -\frac{\pi\sqrt{\beta}}{2}\end{cases}$$

$$\sigma \approx \frac{4}{k}\left(\sin^2\frac{\pi\sqrt{\beta}}{2} + \sum_{l\neq 0, l=-\infty}^{\infty}\sin^2\frac{\pi\beta}{4|l|}\right) \approx \frac{4}{k}\left(\frac{\pi^2\beta}{4} - \frac{\pi^4\beta^2}{48} + 2\sum_{l=1}^{\infty}\left(\frac{\pi\beta}{4l}\right)^2\right) = \frac{\pi^2\beta}{k}$$

$$\sigma = \frac{\pi^2\beta}{k} + O(\beta^3)$$

Now, for $\beta \gg 1 \qquad \Rightarrow$

$$\delta_l = \frac{\pi}{2}(|l| - \sqrt{l^2+\beta})$$

Сечение рассеяния:

$$\sigma = \frac{4}{k}\sum_{l=-\infty}^{\infty}\sin^2\left(\frac{\pi}{2}(|l| - \sqrt{l^2+\beta})\right) \approx \frac{8}{k}\int_0^{\infty} dl\sin^2\left(\frac{\pi}{2}(l - \sqrt{l^2+\beta})\right)$$

$u := \frac{\pi}{2}(l - \sqrt{l^2+\beta})$, $l = \frac{u}{\pi} - \frac{\beta\pi}{4u}$, $\sqrt{l^2+\beta} = -\frac{u}{\pi} - \frac{\beta\pi}{4u}$, $du = \frac{\pi}{2}dl(1 - l/\sqrt{l^2+\beta}) \Rightarrow$

$$\sigma = \frac{8}{k}\int_{-\sqrt{\beta}}^{0} du\left(\frac{1}{\pi} + \frac{\pi\beta}{4u^2}\right)\sin^2 u \approx \frac{8}{k}\left(\frac{1}{\pi}\frac{\sqrt{\beta}}{2} + \frac{\pi\beta}{4}\frac{\pi}{2} + O(1)\right) = \frac{\pi^2\beta}{k} + O(\sqrt{\beta})$$

since

```
Integrate[Sin[ u ]^2, {u, -a, 0}]
Integrate[Sin[ u ]^2/u^2, {u, -a, 0}, Assumptions -> Re[a] > 0 && Im[a] == 0]
```

and for $\beta \gg 1$ we have $\sqrt{\beta} \gg \sin\beta$, and the sine integral $\approx \pi/2$.

$$\sigma = \frac{\pi^2\beta}{k} + O(\sqrt{\beta})$$

В разных предельных случаях получился одинаковый ответ. Возможно, что при любых β ответ

$$\sigma = \frac{\pi^2\beta}{k}$$

Solution. через формулу Борна (???)

(для меня естественно было просто применить обычный формализм Борна для 2д для этого потенциала. Но я не могу найти примеры этого применения, чтобы сделать так же. Также я не уверен в основной формуле, что там фурье образ берем от потенциала, потому что она выведена для 3д случая. нужно тоже посидеть, проверить вывод. возможно, там чуть другая основная формула будет. также есть статьи про это. Рыться во всем этом - время, пока этим не занимался, итак есть, о чем подумать.)

Что по поводу больших порядков?

(сокращаются ли они там тоже? не знаю, не до этого вообще)

ПТФ-14.з3 Парциальное сечение на твёрдом шаре (30 б).

Найдите точное выражение для произвольного парциального сечения рассеяния на твёрдом шаре σ_l. Исследуйте полученную формулу в следующих предельных случаях:
- Оцените вклад p-канала для рассеяния медленных частиц;
- Определите полное сечение рассеяния для быстрых частиц.

Solution.

Уравнение Шрёдингера для радиальной компоненты волновой функции:

$$R''_{kl}(r) + \frac{2}{r}R'_{kl}(r) + \left(k^2 - \frac{l(l+1)}{r^2}\right)R_{kl}(r) = 0$$

Введём замену $R_{kl}(r) = \frac{Q_{kl}(r)}{\sqrt{r}}$.

$$R'_{kl}(r) = \frac{Q'_{kl}(r)}{\sqrt{r}} - \frac{Q_{kl}(r)}{2r^{\frac{3}{2}}}, \quad R''_{kl}(r) = \frac{Q''_{kl}(r)}{\sqrt{r}} - \frac{Q'_{kl}(r)}{r^{\frac{3}{2}}} + \frac{3Q_{kl}(r)}{4r^{\frac{5}{2}}}$$

$$\frac{Q''_{kl}(r)}{\sqrt{r}} - \frac{Q'_{kl}(r)}{r^{\frac{3}{2}}} + \frac{3Q_{kl}(r)}{4r^{\frac{5}{2}}} + \frac{2Q'_{kl}(r)}{r^{\frac{3}{2}}} - \frac{Q_{kl}(r)}{r^{\frac{5}{2}}} + \left(k^2 - \frac{l(l+1)}{r^2}\right)\frac{Q_{kl}(r)}{\sqrt{r}} = 0$$

$$Q''_{kl}(r) + \frac{Q'_{kl}(r)}{r} - \frac{Q_{kl}(r)}{4r^2} + \left(k^2 - \frac{l(l+1)}{r^2}\right)Q_{kl}(r) = 0$$

$$Q''_{kl}(kr) + \frac{Q'_{kl}(kr)}{kr} + \left(1 - \frac{(l+\frac{1}{2})^2}{(kr)^2}\right)Q_{kl}(kr) = 0$$

Получилось уравнение Бесселя с положительной энергией.

$$Q_{kl}(kr) = C_1 J_{l+\frac{1}{2}}(kr) + C_2 Y_{l+\frac{1}{2}}(kr)$$

Граничное условие:

$$Q_{kl}(ka) = 0 \to \frac{C_2}{C_1} = -\frac{J_{l+\frac{1}{2}}(ka)}{Y_{l+\frac{1}{2}}(ka)}$$

Асимптотика при $kr \gg 1$:

$$J_{l+\frac{1}{2}}(kr) \approx \sqrt{\frac{2}{\pi kr}} \cos\left(kr - \frac{\pi(l+\frac{1}{2})}{2} - \frac{\pi}{4}\right) = \sqrt{\frac{2}{\pi kr}} \sin\left(kr - \frac{\pi l}{2}\right)$$

$$Y_{l+\frac{1}{2}}(kr) \approx \sqrt{\frac{2}{\pi kr}} \sin\left(kr - \frac{\pi(l+\frac{1}{2})}{2} - \frac{\pi}{4}\right) = -\sqrt{\frac{2}{\pi kr}} \cos\left(kr - \frac{\pi l}{2}\right)$$

$$Q_{kl}(kr) \approx C\sqrt{\frac{2}{\pi kr}} \sin\left(kr - \frac{\pi l}{2} + \delta_l\right)$$

$$\tan\delta_l = -\frac{C_2}{C_1} = \frac{J_{l+\frac{1}{2}}(ka)}{Y_{l+\frac{1}{2}}(ka)}$$

$$\sin^2\delta_l = \frac{J^2_{l+\frac{1}{2}}(ka)}{J^2_{l+\frac{1}{2}}(ka) + Y^2_{l+\frac{1}{2}}(ka)}$$

$$\sigma_l = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l = \frac{4\pi(2l+1)}{k^2} \frac{J^2_{l+\frac{1}{2}}(ka)}{J^2_{l+\frac{1}{2}}(ka) + Y^2_{l+\frac{1}{2}}(ka)}$$

Рассмотрим предельные случаи:

• Медленные частицы $ka \ll 1$.

Асимптотика функций Бесселя и Неймана:

$$J_{l+\frac{1}{2}}(ka) \approx \frac{1}{\Gamma(l+\frac{3}{2})}\left(\frac{ka}{2}\right)^{l+\frac{1}{2}}, \quad Y_{l+\frac{1}{2}}(ka) \approx -\frac{\Gamma(l+\frac{1}{2})}{\pi}\left(\frac{2}{ka}\right)^{l+\frac{1}{2}}$$

Вклад p-канала:

$$\sigma_1 = \frac{12\pi}{k^2} \frac{\frac{1}{\Gamma(\frac{5}{2})^2}\left(\frac{ka}{2}\right)^3}{\frac{1}{\Gamma(\frac{5}{2})^2}\left(\frac{ka}{2}\right)^3 + \frac{\Gamma(\frac{3}{2})^2}{\pi^2}\left(\frac{2}{ka}\right)^3} \approx \frac{12\pi}{k^2} \frac{\pi^2}{\Gamma(\frac{3}{2})^2\Gamma(\frac{5}{2})^2}\left(\frac{ka}{2}\right)^6 = \frac{12\pi}{k^2}\frac{\pi^2}{\frac{\pi}{4}\frac{9\pi}{16}2^6}k^6a^6$$

$$\sigma_1 = \frac{4\pi}{3}k^4a^6$$

• Быстрые частицы $ka \gg 1$.

Граничное условие:

$$Q_{kl}(ka) \approx C\sqrt{\frac{2}{\pi kr}} \sin\left(ka - \frac{\pi l}{2} + \delta_l\right) = 0 \to ka - \frac{\pi l}{2} + \delta_l = 0$$

$$\delta_l = \frac{\pi l}{2} - ka \to \sin^2\delta_l = \frac{1-\cos 2\delta_l}{2} = \frac{1-(-1)^l\cos 2ka}{2}$$

$$\sigma = \frac{4\pi}{k^2}\sum(2l+1)\sin^2\delta_l \approx \frac{4\pi}{k^2}\int\limits_0^{ka} dl(2l+1)\frac{1-\cos 2ka}{2} \approx \frac{2\pi}{k^2}\int\limits_0^{ka} dl(2l+1) =$$

$$= \frac{2\pi}{k^2}(k^2a^2 + ka) \approx 2\pi a^2$$

$$\sigma = 2\pi a^2$$

ПТФ-14.з4 Рассеяние на потенциале $\sim 1/r^3$ (30 б).

Используя фазовую теорию, найдите сечение рассеяния достаточно быстрых частиц ($kL \gg 1$) на потенциале $V(r) = \frac{L}{2m(r^2+a^2)^{\frac{3}{2}}}$ при дополнительных предположениях:

• В случае $kL \ll \frac{L^2}{a^2}$. *Указание*: параметрически главный вклад в сечение приходит с моментов $l \gg (kL)^{1/3}$. Покажите, что вкладом от моментов $l \ll (kL)^{1/3}$ можно пренебречь.

• В случае $kL \gg \frac{L^2}{a^2}$. *Указание*: вычислите вклад моментов $l \gg (kL)^{1/3}$. Сравните результат с ответом, который получается из Борновского приближения. Применимо ли оно в данном случае?

Solution.

• Случай $kL \ll \frac{L^2}{a^2}$.
Квазиклассическое выражение для фазовых сдвигов:

$$\delta_l = \int\limits_{r_0}^{\infty} dr \left(\sqrt{k^2 - \frac{l(l+1)}{r^2} - 2mV(r)} - k \right) - kr_0 + \frac{\pi l}{2} + \frac{\pi}{4}$$

Разложение:

$$\delta_l = -\int\limits_{r_0}^{\infty} dr \frac{mV(r)}{\sqrt{k^2 - \frac{l(l+1)}{r^2}}}, \quad r_0 = \frac{\sqrt{l(l+1)}}{k} \approx \frac{l}{k}$$

В последнем равенстве использвалось, что $l \gg 1$. Это и то, что $r_0 \gg a$ далее будет показано. При $r \gg a$:

$$V(r) \approx \frac{L}{2mr^3}$$

$$\delta_l = \int\limits_{r_0}^{\infty} dr \frac{L}{2r^3\sqrt{k^2 - \frac{l(l+1)}{r^2}}} = \frac{L}{4l(l+1)} \int\limits_{\frac{l}{k}}^{\infty} \frac{d(k^2 - \frac{l(l+1)}{r^2})}{\sqrt{k^2 - \frac{l(l+1)}{r^2}}} = \frac{Lk}{2l(l+1)} \approx \frac{Lk}{2l^2}$$

$\delta_l \sim 1$ при $kL \sim l^2$. Поскольку частицы достаточно быстрые $kL \gg 1$, то и $l \gg 1$.

$$l^3 \sim lkL \gg kL \to l \gg (kL)^{\frac{1}{3}}$$

Покажем, что $r_0 \gg a$.

$$ka^2 \ll L \to (ka)^2 \ll kL \sim l^2 \to \frac{r_0}{a} = \frac{l}{ka} \gg 1$$

Сечение рассеяния:

$$\sigma = \frac{4\pi}{k^2} \sum_{l=-\infty}^{\infty} (2l+1) \sin^2 \delta_l = \frac{4\pi}{k^2} \int\limits_0^{\infty} dl 2l \sin^2 \frac{Lk}{2l^2} = \frac{\pi^2 L}{4k}$$

$$\sigma = \frac{\pi^2 L}{4k}$$

• Случай $kL \gg \frac{L^2}{a^2}$.
Фазовые сдвиги:

$$\delta_l = \int\limits_{r_0}^{\infty} dr \frac{L}{2(r^2+a^2)^{\frac{3}{2}}\sqrt{k^2 - \frac{l(l+1)}{r^2}}} = \frac{L}{2al} \int\limits_1^{\sqrt{1+(\frac{ka}{l})^2}} \frac{udu}{u^3\sqrt{1+(\frac{ka}{l})^2 - u^2}}, \quad u = 1 + \frac{a^2}{r^2}$$

Сделаем замену $v = \frac{1+(\frac{ka}{l})^2}{u^2} - 1$ и получим

$$\delta_l = \frac{L}{4al} \int\limits_0^{\frac{k^2a^2}{l^2}} \frac{dv}{\sqrt{v}} = \frac{kL}{2(l^2 + k^2a^2)}$$

В борновском приближении:

$$f(\theta) = -\frac{m}{2\pi} \tilde{V}_{\mathbf{k}-\mathbf{k}'} = -\frac{m}{k \sin \frac{\theta}{2}} \int\limits_0^{\infty} dr r \sin \left(2kr \sin \frac{\theta}{2} \right) V(r)$$

$$f(\theta) = -\frac{L}{2k \sin \frac{\theta}{2}} \int\limits_0^{\infty} \frac{r \sin 2kr \sin \frac{\theta}{2}}{(a^2+r^2)^{\frac{3}{2}}} dr \approx L\sqrt{\frac{\pi}{ka \sin \frac{\theta}{2}}} e^{-ka \sin \frac{\theta}{2}}$$

Сечение рассеяния:

$$\sigma = 2\pi \int\limits_0^{\pi} |f(\theta)|^2 \sin \theta d\theta = 2\pi \int\limits_0^{\pi} L^2 \frac{\pi e^{-2ka \sin \frac{\theta}{2}}}{ka \sin \frac{\theta}{2}} \sin \theta d\theta \approx \frac{2\pi^2 L^2}{ka} \int\limits_0^{\pi} \frac{e^{-ka\theta}}{\frac{\theta}{2}} \theta d\theta$$

$$\sigma = \frac{4\pi^2 L^2}{k^2 a^2}$$

LL3-34.1 Разложение волны

Разложить плоскую волну по волновым функциям состояний с определенными значениями проекции m момента на ось y и проекцией p_y импульса на ту же ось.

Solution.

По идее математическая подготовка должна быть такой, чтобы это решение было очевидным. (! допишу это!)

Введем цилиндрическую систему координат y, ρ, φ с осью вдоль оси y. Волновые функции указанных состояний будут иметь вид $Q_m(\rho)e^{im\varphi}e^{ip_y y/\hbar}$. Если отсчитывать угол φ от оси z, разложение можно записать в виде:

$$e^{ikz} = e^{ik\rho\cos\varphi} = \sum_{m=-\infty}^{\infty} Q_m(\rho)e^{im\varphi}$$

(в данном случае $p_y = 0$), откуда

$$Q_m(\rho) = \frac{1}{2\pi}\int_0^{2\pi} \exp[i(k\rho\cos\varphi - m\varphi)]d\varphi = i^m J_m(k\rho)$$

где $J_m(x)$ - функция Бесселя. При $k\rho \gg 1$ для Q_m справедливо асимптотическое выражение:

$$Q_m(\rho) \approx i^m\sqrt{\frac{2}{\pi k\rho}}\sin\left[k\rho - \frac{\pi}{2}\left(m - \frac{1}{2}\right)\right]$$

17.3.12 Problems about partial-wave analysis 2

GKKG.13.18 Phase shifts formula

Obtain an expression for phase shifts directly from the partial-wave expansion of the Born scattering amplitude in a spherically-symmetric potential.

Solution

Let us use the expansion:

$$\frac{\sin qr}{qr} = \frac{\sin\sqrt{2k^2r^2 - 2k^2r^2\cos\theta}}{\sqrt{2k^2r^2 - 2k^2r^2\cos\theta}} = \frac{\pi}{2kr}\sum_{l=0}^{\infty}(2l+1)\left[J_{l+1/2}(kr)\right]^2 P_l(\cos\theta)$$

which follows from the addition theorem for cylindrical functions, if we note that $(\sin z)/z = \sqrt{\pi/2z}J_{1/2}(z)$. Substituting this into Eq. (XIII.8), we obtain the Born amplitude in the form of a series:

$$f^B = \sum_{l=0}^{\infty}(2l+1)\left\{-\frac{\pi m}{\hbar^2 k}\int_0^{\infty} U(r)\left[J_{l+1/2}(kr)\right]^2 rdr\right\}P_l(\cos\theta) \tag{1}$$

Comparing this to expansion $f(k,\theta) = \sum\limits_{l=0}^{\infty}(2l+1)\varphi_l(E)P_l(\cos\theta)$; $\varphi_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k(\cot\delta_l - i)}$ of the scattering amplitude in partial waves, we conclude that the Born approximation corresponds to small scattering phaseshifts, [325] $|\delta_l(k)| \ll 1$, where

$$f = \sum_l (2l+1)\frac{e^{2i\delta_l}-1}{2ik}P_l(\cos\theta) \approx \sum_l (2l+1)\frac{\delta_l(k)}{k}P_l(\cos\theta) \tag{2}$$

From a comparison between Eqs. (1) and (2), we reproduce the known expression for the Born phase shifts - Eq. (XIII.12) - which is a linear-in-the-potential term in the expansion for $\delta_l(k)$.

GKKG.13.19 Phase shifts in $1/r^2$

Find phase shifts in the field $U(r) = \alpha/r^2, \alpha > 0$.

Perform summation of the series $f(k,\theta) = \sum_{l=0}^{\infty}(2l+1)\varphi_l(E)P_l(\cos\theta)$; $\varphi_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k(\cot\delta_l - i)}$, i.e., of the partial-wave expansion of the scattering amplitude for the following cases:
a) $m\alpha/\hbar^2 \ll 1$ for an arbitrary scattering angle;
b) $m\alpha/\hbar^2 \gtrsim 1$ for small-angle scattering;
c) $m\alpha/\hbar^2 \gg 1$ for the backward scattering ($\theta = \pi$).

Find the differential scattering cross-section and compare it to that in the Born approximation and the scattering cross-section that follows from classical mechanics.

[325] The smallness of all phase shifts is a necessary (but not sufficient) condition for the Born approximation to remain valid. This smallness is responsible for the scattering amplitude being real in this approximation.

Solution

Writing the wavefunctions as $\psi_{klm} = u_{kl}(r)Y_{lm}/\sqrt{r}$, for the function $u_{kl}(r)$ we have the following equation (compare to Eq. (IV.6)):

$$u''_{kl} + \frac{1}{r}u'_{kl} + \left\{k^2 - \frac{1}{r^2}\left[\left(l+\frac{1}{2}\right)^2 + \frac{2m\alpha}{\hbar^2}\right]\right\}u_{kl} = 0$$

Its solution, satisfying the boundary condition $u(0) = 0$, is $u_{kl} = CJ_\nu(kr)$, where J_ν is the Bessel function with the index

$$\nu = \sqrt{\left(l+\frac{1}{2}\right)^2 + \frac{2m\alpha}{\hbar^2}}$$

The asymptote of this solution for $r \to \infty$ is

$$u_{kl} \approx C\sqrt{\frac{2}{\pi kr}}\sin\left[kr - \frac{\pi\nu}{2} + \frac{\pi}{4}\right] \equiv C\sqrt{\frac{2}{\pi kr}}\sin\left[kr - \frac{\pi l}{2} + \delta_l\right]$$

The phase shifts are

$$\delta_l = -\frac{\pi}{2}\left[\sqrt{\left(l+\frac{1}{2}\right)^2 + \frac{2m\alpha}{\hbar^2}} - \left(l+\frac{1}{2}\right)\right] \tag{1}$$

Since δ_l does not depend on k, then according to Eq. $f(k,\theta) = \sum_{l=0}^{\infty}(2l+1)\varphi_l(E)P_l(\cos\theta)$; $\varphi_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k(\cot\delta_l - i)}$ the scattering amplitude has the form $f(k,\theta) = F(\theta)/k$, and the differential scattering cross-section goes as $d\sigma/d\Omega \propto k^{-2} \propto E^{-1}$. The same energy-dependence [326] (but not a dependence on the scattering angle) occurs in classical mechanics (see Eq. (5)).

Let us consider some special cases where it is possible (approximately) to sum the series $f(k,\theta) = \sum_{l=0}^{\infty}(2l+1)\varphi_l(E)P_l(\cos\theta)$; $\varphi_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k(\cot\delta_l - i)}$ with phase shifts (1).
a) In the case $m\alpha/\hbar^2 \ll 1$, according to (1) we have

$$\delta_l \approx -\frac{\pi m\alpha}{(2l+1)\hbar^2}$$

where $|\delta_l| \ll 1$. Expanding $e^{2i\delta_l}$ in Eq. $f(k,\theta) = \sum_{l=0}^{\infty}(2l+1)\varphi_l(E)P_l(\cos\theta)$; $\varphi_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k(\cot\delta_l - i)}$, we obtain [327]

$$f(E,\theta) \approx -\frac{\pi m\alpha}{\hbar^2 k}\sum_{l=0}^{\infty}P_l(\cos\theta) = -\frac{\pi m\alpha}{2\hbar^2 k\sin(\theta/2)} \tag{3}$$

[326] For the potential $U = \alpha/r^2$, the dependence $d\sigma/d\Omega \propto E^{-1}$, both in classical and in quantum mechanics, is easily obtained from a dimensional analysis.

[327] To sum this series, use the generating function of the Legendre polynomials (with $z = \cos\theta$ and $x = 1$):

$$\frac{1}{\sqrt{1-2xz+x^2}} = \sum_{l=0}^{\infty} x^l P_l(z)$$

which coincides with the result of the Born approximation (see Problem 13.1 d). The angular dependence of the differential cross-section,

$$\frac{d\sigma}{d\Omega} = |f|^2 = \frac{\pi^2 m\alpha^2}{8\hbar^2 E \sin^2(\theta/2)} \tag{4}$$

is dissimilar from the corresponding result of classical mechanics:

$$\left(\frac{d\sigma}{d\Omega}\right)_{cl} = \frac{\pi^2\alpha(\pi-\theta)}{E\theta^2(2\pi-\theta)^2\sin\theta} \tag{5}$$

b) In the case $m\alpha/\hbar^2 \gtrsim 1$, it is impossible to perform summation of the partial-wave series for an arbitrary scattering angle. But it is easy to see that for sufficiently small scattering angles, Eqs. (3) and (4) are valid. It is connected to an unbounded increase of the scattering amplitude for $\theta \to 0$. Since each term of series $f(k,\theta) = \sum\limits_{l=0}^{\infty}(2l+1)\varphi_l(E)P_l(\cos\theta)$; $\varphi_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k(\cot\delta_l - i)}$ is bounded, then such a divergence of the amplitude means that there are a lot of terms with large values of l in the sum (generally, the smaller the scattering angles, the larger the values of l). But for values of l large enough, relation (2) is still valid, from which Eq. (3) and (4) are deduced. The fact that for small scattering angles, the Born approximation is applicable independently of the value of $m\alpha/\hbar^2$, is reasonable: In the conditions of the problem, large distances contribute dominantly to the relevant quantities (due to the aforementioned divergence of the scattering amplitude), where $U = \alpha/r^2 \ll \hbar v/r$, and the potential can be considered as a perturbation.
c) Let us consider backward scattering. In this case, we have:

$$\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta) = 4\delta(1-\cos\theta)$$

i.e., for $\theta \neq 0$ the sum is equal to zero, and $P_l(-1) = (-1)^l$. Now series $f(k,\theta) = \sum\limits_{l=0}^{\infty}(2l+1)\varphi_l(E)P_l(\cos\theta)$; $\varphi_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k(\cot\delta_l - i)}$ takes the form:

$$f(E,\theta=\pi) = \frac{1}{2k}\sum_{l=0}^{\infty}(2l+1)\exp\left\{-i\pi\sqrt{\left(l+\frac{1}{2}\right)^2 + \frac{2m\alpha}{\hbar^2}}\right\} \tag{6}$$

In the case of $m\alpha/\hbar^2 \gg 1$, the dominant role in this sum is played by the terms with large angular momenta [328] $l \lesssim \left(m\alpha/\hbar^2\right)^{1/4}$. Here, the neighboring terms differ from one another only slightly, and the summation could be replaced by an integration:
$$

$$f(E,\pi) \approx \frac{1}{k}\int_0^{\infty} l\exp\left\{-i\pi\sqrt{l^2+\frac{2m\alpha}{\hbar^2}}\right\}dl \tag{7}$$

$$
Using the substitution $x = \sqrt{l^2 + 2m\alpha/\hbar^2}$, we finally obtain

$$f(E,\pi) = -i\frac{\sqrt{2m\alpha}}{\pi\hbar k}\exp\left\{-i\pi\sqrt{\frac{2m\alpha}{\hbar^2}}\right\} \tag{8}$$

This differential scattering cross-section for $\theta = \pi$ coincides with result (5) of classical mechanics. This remains so also for the region of scattering angles (which expand with an increase of α), that are close to $\theta = \pi$.

Let us note in conclusion that in the case of an attractive potential, $\alpha < 0$, the phase shifts, (1), could become imaginary. Formally, this coincides with the appearance of "absorption" in the system. This instability can be linked to the classical phenomenon of "fall into the center" (see Problem 9.14). What concerns the small-angle scattering, it is described by Eqs. (3) and (4), independently of the sign of α.

[0] [328] For large values of l, terms of the sum (6) oscillate quickly, and as result of their mutual compensation, the corresponding part of the sum becomes small. Let us note that for the calculation of series (6), as well as for the previous sum with the δ-function, we should introduce a cutoff factor, $e^{-\gamma l}$ with $\gamma > 0$, in integral (7), and then the limit take $\gamma \to 0$ in the final result.

GKKG.13.20 Scattering on a zero-range potential

Find the wavefunction, $\psi^+_{\mathbf{k}_0}(\mathbf{r})$, scattering amplitude, and scattering cross-section of a particle in a zero-range potential (see Problem 4.10). Find the value of effective radius, r_0.

Solution

Since a zero-range potential affects only particles with the angular momentum $l = 0$, then only an s-scattering phase-shift, $\delta_0(k)$, is non-zero, and the scattering amplitude does not depend on the angle θ. The asymptotic form of the wavefunction,

$$\psi^+_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{f(E)}{r}e^{ikr} \tag{1}$$

determines the exact solution of the Schrdinger equation for all $r > 0$. Comparing the wavefunction expansion for $r \to 0$,

$$\psi^+_{\mathbf{k}} \approx \frac{f}{r} + (1 + ikf)$$

with the boundary condition for the zero-range potential (see Problem 4.10), we find

$$f(E) = -\frac{a_0}{1 + ika_0}, \quad \sigma = 4\pi|f|^2 = \frac{4\pi}{k}\,\mathrm{Im}\, f(E) = \frac{4\pi a_0^2}{1 + k^2a_0^2} \tag{2}$$

Here, $a_0 = 1/\alpha_0$. Note that $f(0) = -a_0$, where a_0 is the scattering length of a z.r.p.

Finally, using the equality $e^{2i\delta} - 1 = 2i/(\cot\delta - i)$, we obtain the s-scatterig phaseshift on the zero-range potential as follows:

$$k\cot\delta_0(k) = -\frac{1}{a_0} \tag{3}$$

Its comparison with the effective-range expansion, (XIII.15), proves that for scattering from a z.r.p., the effective radius of interaction is $r_0 = 0$.

GKKG.13.21 Reconstruct the interaction potential

Reconstruct the interaction potential $U(r)$ from the s-scattering phase-shift $\delta_0(k)$, considering it to be known for all energies, and assuming that $|\delta_0(k)| \ll 1$.

To illustrate applications of this result, consider the following dependencies:

a) $\delta_0(k) = \mathrm{const}$;

b) $\delta_0(k) = \frac{\alpha k}{1+\beta k^2}$.

Solution

(в теории уже раздел создан, по идее им это должно решаться, но пока я)

Since $|\delta_0(k)| \ll 1$ for all energies, we can consider the potential as a perturbation and use expression (XIII.12) for the phase shift of the s-wave:

$$\delta_0(k) = -\frac{2m}{\hbar^2 k}\int\limits_0^\infty U(r)\sin^2 krdr = -\frac{m}{\hbar^2 k}\int\limits_0^\infty U(r)[1 - \cos 2kr]dr \tag{1}$$

Multiplying both parts of this equality by $\left(-\hbar^2 k/2m\right)$ and differentiating by k, we obtain

$$-\frac{\hbar^2}{2m}\frac{d}{dk}\left[k\delta_0(k)\right] = \int\limits_0^\infty rU(r)\sin 2krdr \equiv \frac{i}{2}\int\limits_{-\infty}^\infty rU(|r|)e^{-2ikr}dr \tag{2}$$

Here we have used the even continuation of the potential, $U(-|r|) \equiv U(|r|)$, into the region with negative values of r.

Equation (2) determines the Fourier component of the potential (to be more precise, of the function $rU(|r|)$) and allows us to find the potential using the inverse Fourier transform:

$$rU(|r|) = \frac{i\hbar^2}{\pi m}\int\limits_{-\infty}^\infty e^{2ikr}\frac{d}{dk}\left[k\delta_0(k)\right]dk \tag{3}$$

Since according to Eq. (1), $\delta_0(k)$ is an odd function of the variable k, and so $\delta_0'(k)$ is an even function, then Eq. (3) takes the form:

$$U(r) = -\frac{2\hbar^2}{\pi m r}\int\limits_0^\infty \sin(2kr)\frac{d}{dk}\left[k\delta_0(k)\right]dk \tag{4}$$

Let us consider applications of this general formula.
a) In the case of $\delta_0(k) = \text{const} = C$ (for $k > 0$), according to Eq. (4) we obtain:

$$U(r) = -\frac{2\hbar^2 C}{\pi m r}\int\limits_0^\infty \sin 2kr dk = -\frac{\hbar^2 C}{\pi m r^2} \equiv \frac{\gamma}{r^2} \tag{5}$$

To calculate this integral, introduce the "cutoff" factor $e^{-\lambda k}$ with $\lambda > 0$, and in the final result take $\lambda \to 0$.
b) Substituting $[k\delta_0(k)]' = 2\alpha k/\left(1+\beta k^2\right)^2$ into Eq. (3) and calculating the integral using residues, we find:

$$U(r) = -\frac{2\alpha\hbar^2}{m\sqrt{\beta^3}}\exp\left\{-\frac{2r}{\sqrt{\beta}}\right\} \equiv U_0 e^{-r/R} \tag{6}$$

Note that the condition $|\delta_0(k)| \ll 1$ assumes that $|C| \ll 1$ and $|\alpha| \ll \sqrt{\beta}$. The reconstructed potentials (5) and (6), as expected, are consistent with the applicability condition of the Born approximation for any energy.

GKKG.13.22 Phase shifts for an exchange potential

Obtain phase shifts in the Born approximation for an exchange potential (see Problem 13.3).

Solution

Since the action of the operator $\hat{U}_{ex}$ on the wavefunction of a state with a definite value of angular momentum, l, is reduced to its multiplication by $(-1)^l U(r)$, then the expression for the phase shift, $\delta^B_{ex,l}(k)$, differs from the Born expression, (XIII.12), for a regular potential, $U(r)$, only by the factor $(-1)^l$.

GKKG.13.24 Scattering in symmetric magnetic field

Using the partial-wave decomposition, find the scattering amplitude and differential scattering cross-section of charged particles in an axially symmetric magnetic field, $\mathcal{H}(\rho)$, directed along the z axis and localized at small distances $\rho \le a$ in the vicinity of this axis.
Hint: Consider the limiting case $a \to 0$, and a finite value, Φ_0, of the magnetic flux. It is convenient to choose the vector potential in the form $A_\varphi = \Phi_0/2\pi\rho, A_z = A_\rho = 0$.

Solution

In the polar coordinates, the Hamiltonian of transverse motion in a magnetic field $\hat{H}_\perp = (\hat{\mathbf{p}} - e\mathbf{A}/c)^2/2\mu$, takes the form: [330]

$$\hat{H}_\perp = \frac{\hbar^2}{2\mu}\left\{-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\left[\lambda^2 + 2i\lambda\frac{\partial}{\partial\varphi} - \frac{\partial^2}{\partial\varphi^2}\right]\right\} \tag{1}$$

where $\lambda = e\Phi_0/2\pi\hbar c$. Since the operator $\hat{H}_\perp$ commutes with $\hat{l}_z$, the two-dimensional theory of scattering developed in the previous problem is also applicable here. Now, though, the phase shifts, δ_m, depend on the sign of m. The radial functions here, as well as for free motion, are expressed in terms of the Bessel functions, $J_\nu(k\rho)$, but with the index $\nu = |m - \lambda|$. Using their known asymptote, we find

[330] Note that free motion along the field is not particularly interesting and therefore is not being considered. Also note that for to derive Hamiltonian (1), we used the following azimuthal component of the gradient operator, $\rho^{-1}\nabla_\varphi = \partial/\partial\varphi$.

$$\delta_m = -\frac{\pi}{2}(|m-\lambda| - |m|)$$

The scattering amplitude (see Eq. (5) of the previous problem) becomes

$$f(k,\varphi) = \frac{1}{i\sqrt{2\pi k}}\sum_{m=-\infty}^{\infty}\left\{e^{i\pi(m-|m-\lambda|)} - 1\right\}e^{im\varphi} \tag{2}$$

Denoting the minimum value of m (that is still larger than λ) by m_0, and dividing the sum into two pieces: with $m \geq m_0$ and with $m \leq m_0 - 1$, we can calculate the latter summing up a geometrical progression. This yields a closed equation for the amplitude and differential cross-section:

$$f = i\frac{\exp\{i\,(m_0 - 1/2)\,\varphi\}}{\sqrt{2\pi k}}\frac{\sin\pi\lambda}{\sin(\varphi/2)}, \quad \frac{d\sigma}{d\varphi} = \left.\frac{\sin^2(e\Phi_0/2\hbar c)}{2\pi k\sin^2(\varphi/2)}\right|_{\phi\to 0} \propto \phi^{-2}$$

An interesting property of this result is the infinite value of the total scattering cross-section, i.e., particle scattering occurs even for an arbitrarily large impact parameter. From the point of view of classical theory, this conclusion appears counter-intuitive: the magnetic field and the Lorentz force are different from zero only on the axis, and hence have no influence on the particle's classical motion. This paradox is a manifestation of the fact that the phenomenon due to the magnetic flux described in this problem, the Aharonov-Bohm effect, is purely quantum, and disappears in the classical limit; for $\hbar \to 0$ and $k^{-1} = \hbar/p \to 0$, the scattering is indeed absent. In quantum mechanics, the interaction between a charged particle and a magnetic field is characterized by a vector potential: as in the Hamiltonian. [331] In this problem, despite the fact that outside the axis, the field vanishes, $\mathcal{H} = 0$, the vector potential can not be turned off ("gauged away") by any gauge transformation $\left(\oint \mathbf{A}\cdot d\mathbf{l} = \Phi_0\right)$, and its slow, $\propto 1/\rho$, decrease on large distances explains the infinite scattering cross-section.

[331] See also an excellent discussion about whether the vector potential is "real" in The Feynman Lectures on Physics, vol. 6, Ch. 15.

GKKG.13.25 High energy phase shifts

Find the energy dependence of phase shifts, $\delta_l(k)$, with a fixed value of l, in the limit $k \to \infty$. Consider potentials with the following behavior at small distances ($r \to 0$): $U \approx \alpha/r^\nu$ with a) $\nu < 1$; b) $1 < \nu < 2$; c) $\nu = 1$.

Solution

For large energies, the Born approximation is applicable, and we can use expression (XIII.12) for the phase shifts. For $k \to \infty$, the argument of the Bessel function is large, $x = kr \gg 1$, in the entire integration domain, except for a narrow region of small r. Using the known asymptote for $J_\mu(x)$, we obtain

$$\delta_l(k) = -\frac{2m}{\hbar^2 k}\int\limits_0^\infty U(r)\sin^2\left(kr - \frac{\pi l}{2}\right)dr \approx -\frac{m}{\hbar^2 k}\int\limits_0^\infty U(r)dr \propto k^{-1} \tag{1}$$

The fast-oscillating factor $\sin^2(x - \pi l/2)$ was replaced by its mean value, equal to $1/2$. This result is valid in case a), where $rU(r) \to 0$ for $r \to 0$.

For more singular potentials, Eq. (1) is not applicable, due to a divergence of the integral. Such a divergence means that now the region of small r plays a dominant role, and we cannot replace $J_\mu(x)$ by its asymptote. Dividing the integration domain over r in Eq. (XIII.12) into two: from $r = 0$ to some small but finite R, and from $r = R$ to infinity, we see that the second of these integrals is proportional to k^{-1}, as in Eq. (1). A contribution of the first of these integrals is dominant, and we can put there $U = \alpha/r^\nu$. Making substitution $x = kr$, we obtain the [332]

$$\delta_l \approx -\frac{\pi m\alpha}{\hbar^2}k^{\nu-2}\int\limits_0^\infty \frac{J^2_{l+1/2}(x)dx}{x^{\nu-1}} = -\frac{\pi m\alpha}{\hbar^2}\frac{\Gamma(\nu-1)\Gamma(l+(3-\nu)/2)}{2^{\nu-1}\Gamma^2(\nu/2)\Gamma(l+(\nu+1)/2)}k^{\nu-2} \propto k^{\nu-2} \tag{2}$$

Normally, we would replace the upper limit of integration, equal to kR, for $k \to \infty$ by ∞. For $\nu = 1$ however, such a replacement is not valid due to the divergence of the integral (in the upper limit).

Using the asymptote $J_\mu(x)$ for $x \to \infty$, we calculate the divergent part as follows

$$\delta_l \approx -\frac{m\alpha}{\hbar^2 k}\ln kR, \quad \nu = 1 \tag{3}$$

This equation has the logarithmic accuracy in accordance with an uncertainty in the value of R.

Let us note that the ν-dependence of the phase-shifts, $\delta_l(k)$, for $k \to \infty$, affects the scattering of particles with a large momentum transfer. This is connected with the fact that $f^B \propto \tilde{U}(q)$ for large values of q is determined by the singularities of the potential $U(r)$ as a function of r. For singular at $r \to 0$ potentials, $U \approx \alpha/r^\nu$, we have $\tilde{U} \propto q^{\nu-3} \propto k^{\nu-3}$ for $q \to \infty$. But such a difference in the energy dependence of phase-

[332] For $\nu = 2$, the independence of phase-shifts from k holds for any values of α and l, even if the Born approximation is not applicable (see Problem 13.19). Note also that for $\nu > 2$, the Born approximation breaks down.

shifts with fixed values of l does not affect the total scattering cross-section, $\sigma \propto 1/E$, that is determined by angular momenta $l \sim kR \gg 1$.

GKKG.13.26 Born and quasi-classical phase-shifts

Prove that for large values of energy and angular momentum, where $kR \sim l \gg 1$, the Born approximation, (XIII.12), for phase-shifts crosses over to the quasi-classical expression, see Eq. (XIII.14).

Solution

In Eq. (XIII.12) for the values $l \sim kR \gg 1$ (R is the potential radius), we divide the integration domain into two parts: from $r = 0$ to $r = r_0 \equiv (l + 1/2)/k$, and from $r = r_0$ to $r = \infty$. In the second of these integrals, we use the tangent approximation for the Bessel function, i.e., the following asymptote

$$J_\nu\left(\frac{\nu}{\cos\beta}\right) \approx \sqrt{\frac{2}{\pi\nu\tan\beta}}\cos\left(\nu\tan\beta - \beta\nu - \frac{\pi}{4}\right), \quad \nu \gg 1 \tag{1}$$

Here, $\nu = l + 1/2$ and $\nu/\cos\beta = kr$, so that $\nu\tan\beta = k\sqrt{r^2 - r_0^2}$. After replacing the fast-oscillating factor, $\cos^2[\ldots]$, under the integral by its mean value of $1/2$, we find:

$$\delta_l^B(k) \approx -\frac{m}{\hbar^2 k}\int\limits_{r_0}^{\infty}\frac{rU(r)dr}{\sqrt{r^2 - r_0^2}} \tag{2}$$

We restrict ourselves to the second of the integrals mentioned, since the contribution of the first one is small. This smallness is connected to the fact that for $\nu \gg 1$, the function $J_\nu(x)$ decreases exponentially with the decrease of x from the value $x = \nu$. Such a decrease of $J_\nu(x)$ is a manifestation of the common quasiclassical behavior, where the quasiclassical wavefunctions decreases rapidly into a classically-forbidden region, inside a barrier (in this case, the centrifugal barrier).

Equation (2) coincides with the known quasi-classical expression, (XIII.14), for the phase shift in the case of $|U(r)| \ll E$. The use of the Born approximation assumes the fulfilment of a stricter condition, $|U(r)| \ll \hbar v/r$, with $|\delta_l^{B''}| \ll 1$.

According to Eq. (2), a dependence of the phase shift on l and k (in the relevant parameter range) is determined by the expression:

$$\delta_l^B(k) = \frac{g(s)}{k}, \quad s = \frac{l + 1/2}{k} \tag{3}$$

The function $g(s)$ depends on the concrete form of the potential. If the Born approximation applies, by replacing the summation over l with an integration in Eq. $f(k,\theta) = \sum\limits_{l=0}^{\infty}(2l+1)\varphi_l(E)P_l(\cos\theta)$; $\varphi_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k(\cot\delta_l - i)}$, we obtain the known result, $\sigma \propto 1/E$ for $E \to \infty$ (for a short-range potential).

17.3.13 Advanced different problems about typical scatterings

ЛШ-11 Диаграммный ряд и интегральное уравнение для амплитуды рассеяния

Покажите, что рассеяние частицы в статическом внешнем поле $V(\mathbf{r})$ описывается суммой графиков:

Какие выражения надо сопоставлять графическим элементам? (Используйте импульсное представление.)

Свяжите эти диаграммы с амплитудой рассеяния $f(\mathbf{k}_1, \mathbf{k}_2)$. Получите соотношение

$$f(\mathbf{k}_1, \mathbf{k}_2) = -\frac{m}{2\pi\hbar^2}F(\mathbf{k}_1, \mathbf{k}_2)$$

где $F(\mathbf{k}_1, \mathbf{k}_2)$ удовлетворяет уравнению

$$F(\mathbf{k}_1, \mathbf{k}_2) = V(\mathbf{k}_2 - \mathbf{k}_1) + \int\frac{V(\mathbf{k}_2 - \mathbf{q})F(\mathbf{k}_1, \mathbf{q})}{\varepsilon - \hbar^2\mathbf{q}^2/2m + i\delta}\frac{d^3q}{(2\pi)^3},$$

где $\varepsilon = \hbar^2\mathbf{k}_1^2/(2m) = \hbar^2\mathbf{k}_2^2/(2m)$. Определенную так амплитуду $F(\mathbf{k}_1, \mathbf{k}_2)$ называют амплитудой рассеяния в энергетической нормировке.

Пользоваться ею часто бывает удобнее, чем обычной амплитудой рассеяния. Именно такая амплитуда рассеяния естественно возникает в диаграммной технике (см. другие задачи этой главы, а также задачи глав 9 - 11). (???) По сравнению с обычной квантовомеханической амплитудой рассеяния $f(\mathbf{k}_1, \mathbf{k}_2)$, она менее произвольна, поскольку никак не зависит от выбора нормировки плоских волн.

Solution.

Суть в том, что (?!??!?)
(не задача, а кусок важной теории и определения параметров. впишу в 1ю потом!!!)
Мы будем обращаться с функцией Грина несколько более вольно, чем это принято в учебниках по квантовой механике. Перед тем, как читать решение, полезно вспомнить стандартный вывод интегрального уравнения для амплитуды рассеяния, использующий уравнение Шредингера в импульсном представлении (см. [2], §130).
(???? пока его не полностью выучил, потом доработаю!!!)
Чтобы найти состояние рассеяния (3.3),(3.4), запишем уравнение Шредингера для движения в потенциале $V(\mathbf{r})$ через функцию Грина:

$$\hat{G}^{-1}\psi_{\mathbf{k}}(\mathbf{r}) = 0 \quad \text{или} \quad \left(\hat{G}_0^{-1} - \hat{V}\right)\psi_{\mathbf{k}}(\mathbf{r}) = 0.$$

Будем искать решение в виде $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{kr}} + \chi_{\mathbf{k}}(\mathbf{r})$. На массовой поверхности, при $\varepsilon = k^2/2m$, получаем уравнение для $\chi_{\mathbf{k}}(\mathbf{r})$:

$$\left(\hat{G}_0^{-1} - \hat{V}\right)\chi_{\mathbf{k}}(\mathbf{r}) = V|\mathbf{k}\rangle$$

(???? тоже пока не понял этот переход)
Записываем решение через функцию Грина, $\chi_{\mathbf{k}}(\mathbf{r}) = \langle\mathbf{r}|\hat{G}\hat{V}|\mathbf{k}\rangle$, и разлагаем $\hat{G}$ в ряд по $\hat{V}$:

$$\chi_{\mathbf{k}}(\mathbf{r}) = \langle\mathbf{r}|\hat{G}_0\hat{V} + \hat{G}_0\hat{V}\hat{G}_0\hat{V} + ...|\mathbf{k}\rangle.$$

Удобно переписать это выражение, введя оператор

$$\hat{F} = \hat{V} + \hat{V}\hat{G}_0\hat{V} + \hat{V}\hat{G}_0\hat{V}\hat{G}_0\hat{V} + ...$$

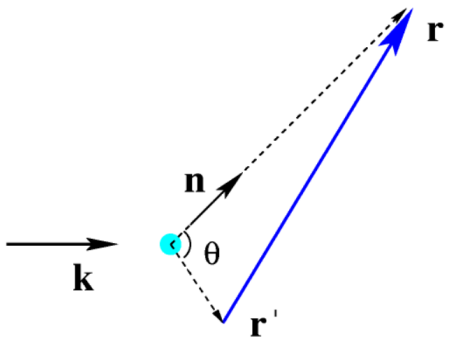
Имеем

$$\chi_{\mathbf{k}}(\mathbf{r}) = \langle\mathbf{r}|\hat{G}_0\hat{F}|\mathbf{k}\rangle.$$

Смысл этой записи в том, что $\hat{F}$ описывает многократное рассеяние падающей волны на потенциале $V(\mathbf{r})$, а $\hat{G}_0$ - свободное движение после последнего рассеяния.
В координатном представлении G_0 имеет вид:

$$G_0(\varepsilon, \mathbf{r}, \mathbf{r}') = \int \frac{e^{i\mathbf{p}(\mathbf{r}-\mathbf{r}')}}{\varepsilon - \mathbf{p}^2/2m + i\delta}\frac{d^3p}{(2\pi)^3} = -\frac{m}{2\pi\hbar^2}\frac{e^{i\varkappa|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|},$$

где $\hbar\varkappa = \sqrt{2m\varepsilon}$. На массовой поверхности $\varkappa = k$. Здесь в знаменателе слагаемое $i\delta$ введено для того, чтобы выбрать запаздывающее решение. С тем же успехом можно было бы выбрать знак $-i\delta$, что привело бы к ряду для $f^*(\mathbf{k}', \mathbf{k})$. Комплексно-сопряженная амплитуда соответствует опережающему решению задачи о рассеянии.
Нас интересует асимптотика $\chi(\mathbf{r})$, поэтому запишем $\mathbf{r} = R\mathbf{n}$ и будем считать R большим. Тогда $|\mathbf{r}-\mathbf{r}'| = R - |\mathbf{r}'|\cos\theta + O(1/R)$, где θ - угол между $\mathbf{n}$ и $\mathbf{r}'$



Подставляем G_0 и разлагаем $|\mathbf{r}-\mathbf{r}'|$:

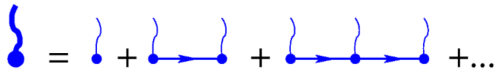
$$\chi(\mathbf{r}) = -\frac{m}{2\pi\hbar^2}\frac{e^{i\varkappa R}}{R}\int e^{-i\varkappa|\mathbf{r}'|\cos\theta}\langle\mathbf{r}'|F|\mathbf{k}\rangle d^3r'.$$

Сравнивая этот ответ с определением амплитуды рассеяния, получаем требуемое соотношение:

$$f(\mathbf{k}_1, \mathbf{k}_2) = -\frac{m}{2\pi\hbar^2}\langle\mathbf{k}_2|\hat{F}|\mathbf{k}_1\rangle$$

где $\mathbf{k}_2 = |k_1|\mathbf{n}$.

Перейдем к выводу интегрального уравнения. Ряд для $\hat{F}$ может быть представлен графически, как показано на рис.



Запишем сумму

$$F = \hat{V} + \hat{V}\hat{G}_0\hat{V} + \hat{V}\hat{G}_0\hat{V}\hat{G}_0\hat{V} + ...$$

в импульсном представлении:

$$F(\mathbf{k}_1, \mathbf{k}_2) = F^{(1)}(\mathbf{k}_1, \mathbf{k}_2) + F^{(2)}(\mathbf{k}_1, \mathbf{k}_2) + ...,$$

где

$$F^{(1)}(\mathbf{k}_1, \mathbf{k}_2) = V(\mathbf{k}_2 - \mathbf{k}_1),$$

$$F^{(2)}(\mathbf{k}_1, \mathbf{k}_2) = \int \frac{V(\mathbf{k}_2 - \mathbf{q})\, V(\mathbf{q} - \mathbf{k}_1)\left(d^3q\right)}{\varepsilon - \mathbf{q}^2/(2m) + i\delta},$$

$$\cdots\cdots\cdots\cdots\cdots\cdots$$

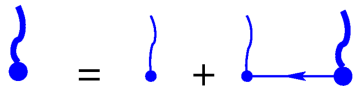
$$F^{(n)}(\mathbf{k}_1, \mathbf{k}_2) = \int ... \int \frac{V(\mathbf{k}_2 - \mathbf{q}_{n-1}) ... V(\mathbf{q}_1 - \mathbf{k}_1)\left(d^3q_{n-1}\right) ... \left(d^3q_1\right)}{\left(\varepsilon - \mathbf{q}_{n-1}^2/(2m) + i\delta\right) ... \left(\varepsilon - \mathbf{q}_1^2/(2m) + i\delta\right)},$$

где $\left(d^3q_i\right) = d^3q_i/(2\pi)^3, \varepsilon = \hbar^2\mathbf{k}_1^2/(2m)$.

Связь этих выражений с рядом выше очевидна: волнистым линиям соответствуют матричные элементы потенциала, прямым линиям — функции Грина. По всем внутренним импульсам надо проинтегрировать, а входящий и выходящий импульсы взять на массовой поверхности. Получаем интегральное уравнение для $\hat{F}$:

$$\begin{aligned}\hat{F} &= \hat{V} + \hat{V}\hat{G}_0\hat{V} + \hat{V}\hat{G}_0\hat{V}\hat{G}_0\hat{V} + ... = \\ &= \hat{V} + \hat{V}\hat{G}_0\left(\hat{V} + \hat{V}\hat{G}_0\hat{V} + ...\right) \\ &= \hat{V} + \hat{V}\hat{G}_0\hat{F}\end{aligned}$$

Графически это можно изобразить так:



В импульсном представлении интегральное уравнение принимает вид

$$F(\mathbf{k}_1, \mathbf{k}_2) = V(\mathbf{k}_2 - \mathbf{k}_1) + \frac{2m}{\hbar^2}\int \frac{V(\mathbf{k}_2 - \mathbf{q})\, F(\mathbf{k}_1, \mathbf{q})}{k_1^2 - q^2 + i\delta}\frac{d^3q}{(2\pi)^3}.$$

Решая это уравнение последовательными приближениями, вновь получаем ряд для $\hat{F}$.

(??? окей, вроде идейно все понятно, нашел уравнения, теперь понять нужно, как их решать???? также пока не готов самостоятельно это вывести, тут еще нужно тренироваться!)

ЛШ-12 Слабо связанное состояние в мелкой яме (!!)

(типичная задача, среди первых перенесу или в теорию)

Мелкая яма - яма, глубина которой $U_0 \ll \hbar^2/2ma^2$, где a - радиус ямы. Размер связанного состояния в такой яме много больше ее радиуса, а энергия связи - много меньше глубины ямы U_0. Рассмотрим мелкую яму в пространстве произвольной размерности D, и выясним, в каких случаях в ней может образоваться связанное состояние.

Решите эту задачу, используя связь амплитуды рассеяния со связанными состояниями $F(\mathbf{k}_1, \mathbf{k}_2) = V(\mathbf{k}_2 - \mathbf{k}_1) + \int \frac{V(\mathbf{k}_2 - \mathbf{q})F(\mathbf{k}_1, \mathbf{q})}{\varepsilon - \hbar^2\mathbf{q}^2/2m + i\delta}\frac{d^3q}{(2\pi)^3}$. Энергия каждого связанного состояния соответствует полюсу амплитуды $F(\mathbf{k}_1, \mathbf{k}_2)$ как функции энергии ε. Покажите, что связанное состояние в мелкой яме существует только при $D \leqslant 2$.

Воспользуйтесь тем, что в пространстве размерности D амплитуда $F(\mathbf{k}_1, \mathbf{k}_2)$ удовлетворяет аналогичному уравнению, только при $d^3q/(2\pi)^3 \to d^Dq/(2\pi)^D$. В уравнении (3.13) замените потенциал ямы на δ-функцию - при этом все интегрирования по импульсам станут независимыми.

Сравните результаты, получающиеся при $D = 1, 2$, с известными квантовомеханическим выражениями (см. задачи в ЛЛ3 пар 45)

(??? кст, почему я их еще не знаю, выпишу их!???)

Смысл и обзор решения 12.

Полюсы функции Грина $\hat{G}(\varepsilon)$ дают спектр системы.
(?? в теории плохо это прописано, не глубоко понимаю это утверждение ещё. допишу в теорию!!)
При этом, поскольку $\hat{G}$ и $\hat{F}$ связаны соотношением $\hat{G} = \hat{G}_0 + \hat{G}_0\hat{F}\hat{G}_0$, каждому связанному состоянию отвечает полюс $\hat{F}(\varepsilon)$.

Размерность $D = 1$

Начнем со случая $D = 1$. Рассмотрим одномерную яму глубины U_0 и ширины a. Заменяя потенциал на δ-функцию $V(x) = -U_0 a\delta(x)$, получаем фурье-компоненту $V(q) = -U_0 a = \text{const}$. При этом уравнение для $F(k, k')$ принимает вид

$$F(k, k') = -U_0 a + U_0 a \int \frac{F(k, q)}{\varepsilon - q^2/2m + i\delta} \frac{dq}{2\pi}.$$

(???? нужно четко прописать свойства этого уравнения, пока только вывел его в задаче выше, по сути в теории нужно это написать нормально!!)
Видим, что $F(k, k')$ не зависит от k', поэтому

$$F(k) = -U_0 a - \frac{U_0 a}{2\pi} F(k) \int\limits_{-\infty}^{+\infty} \frac{2m dq}{q^2 - k^2 - i\delta},$$

что дает

$$F^{-1} + (U_0 a)^{-1} = -im/k = -i\sqrt{m/2\varepsilon},$$

где $\varepsilon = k^2/(2m)$.
(?? интеграл такой еще не считал, вроде не сложно, но потом пересчитаю!)
Получаем

$$F(\varepsilon) = -\frac{U_0 a\sqrt{2(\varepsilon + i\delta)/m}}{\sqrt{2(\varepsilon + i\delta)/m} + iU_0 a}.$$

(?? нужно проделать, пока не проделал все еще!??!)
Амплитуда рассеяния $F(\varepsilon)$ имеет полюс при $\varepsilon_0 = -mU_0^2 a^2/\left(2\hbar^2\right)$, что совпадает с известным ответом для одномерной δ-ямы.

Размерность $D = 2$

Пусть теперь $D = 2$. Снова считаем фурье-компоненту потенциала независящей от $k : V(k) = -U_0 a^2$. Уравнение для F имеет вид

$$F(\varepsilon) = -U_0 a^2 + U_0 a^2 \frac{2m}{\hbar^2} \int F(\varepsilon) \frac{2\pi q}{q^2 - k^2 - i\delta} \frac{dq}{(2\pi)^2},$$

где F снова есть функция только ε.
Интеграл $\int\limits_0^\infty \frac{dq^2}{q^2 - k^2 - i\delta}$ логарифмически расходится на верхнем пределе. Но это не страшно: при $q \geqslant a^{-1}$ фурье-компонента $V(k)$ начинает быстро осциллировать, и интеграл с $V(k)$ сходится. Следовательно, можно пользоваться выражением (3.33), обрезав его “вручную” при $q \approx a^{-1}$:

$$\int\limits_0^{a^{-2}} \frac{dq^2}{q^2 - k^2 - i\delta} = \pi i + \ln \frac{1}{a^2 (k^2 + i\delta)}$$

(!!!! это полный бред, интеграл так не взять. полностью бредовая формула. в теории потом напишу, как делать нормально (пока додумываю))
Итак,

$$F(\varepsilon) \approx -\frac{U_0 a^2}{1 + (2ma^2 U_0/4\pi\hbar^2) \ln(-k^2 a^2)} = -\frac{U_0 a^2}{1 + (mU_0 a^2/2\pi\hbar^2) \ln(-\varepsilon m a^2/\hbar^2)}$$

Дискретный уровень находим как полюс F:

$$\varepsilon_0 \approx -\frac{\hbar^2}{ma^2}\exp\left(-\frac{2\pi h^2}{ma^2U_0}\right).$$

Обратим внимание, что из-за неизвестного множителя порядка единицы, появившегося при обрезании в аргументе логарифма, уровень ε_0 дается выражением (3.36) только по порядку величины.

(??? мы ведь не знаем, где обрезать на самом деле нужно?? почему именно там обрезка идет есть пояснения?)

Размерность $D > 2$

В размерности $D > 2$ интеграл

$$\int_0^{a^{-1}} \frac{q^{D-1}dq}{q^2 - k^2 - i\delta}$$

остается конечным при $k \to 0$. Поэтому для слабого потенциала $F(\varepsilon)$ не имеет полюсов при $|k| \ll a^{-1}$, что означает отсутствие связанного состояния.

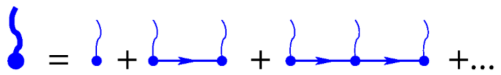
(укажу это в теории. там как-то из каких-то других соображений этот вывод был получен)

ЛШ-13 Двумерное рассеяние: логарифм и ренормгруппа (???)

Рассмотрим подробнее рассеяние в размерности 2 на короткодействующем потенциале. Это может быть яма, причем не обязательно мелкая, или потенциал положительного знака. Определим зависимость амплитуды рассеяния F от энергии в низкоэнергетической области. Нас интересует область энергий много меньших $\varepsilon_a = \hbar^2/2ma^2$, где a - радиус ямы. Ясно, что зависимость от энергии ε возникает от интегрирования по $|q| \ll a^{-1}$.

Для правильного описания низкоэнергетической физики, как и при отыскании связанного состояния, кажется достаточным заменить потенциал на δ-функцию. При этом интегралы по q начинают логарифмически расходиться при $q \to \infty$, и их придется «обрезать руками» при $q \approx a^{-1}$. Такой "ремесленный" подход, хотя и приводит к качественно правильному ответу, является слишком грубым, т.к. полностью игнорирует, например, глубокие уровни в потенциале, если таковые есть.

Более рафинированный метод заключается в следующем. Вычислим производную $\partial F(\varepsilon)/\partial\varepsilon$. Дифференцируя диаграммы рис.



по ε и собирая члены, получим уравнение

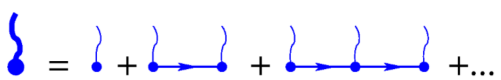
$$\frac{\partial}{\partial\varepsilon}F(\varepsilon) = \frac{m}{2\pi\hbar^2\varepsilon}F^2(\varepsilon),$$

справедливое при $|\varepsilon| \ll \varepsilon_a$. Решив это уравнение, можно связать обрезку логарифма и амплитуду F при большой энергии.

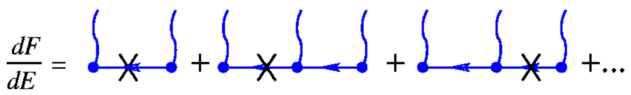
(???? забыли сформулировать, что в задаче то делать? проделать эти вычисления?)

Solution. 13.

Производную $\partial F/\partial\varepsilon$ можно связать с F в общем виде, так, что получится выражение, справедливое при произвольном потенциале. Для этого надо продифференцировать ряд

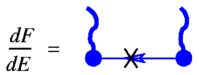


почленно, получим:



$$\text{ } := \frac{\partial}{\partial\varepsilon}G_0 = -\frac{1}{\left(\varepsilon - p^2/2m + i\delta\right)^2} = -G_0^2.$$

Группируя члены графического ряда и пользуясь графическим представлением амплитуды F (жирными линиями), находим:



(??? проверю!)
Отсюда:

$$\frac{\partial}{\partial\varepsilon}F_\varepsilon\left(k_1,k_2\right) = -\int \frac{F_\varepsilon\left(k_1,q\right)F_\varepsilon\left(q,k_2\right)}{\left(\varepsilon - q^2/2m + i\delta\right)^2}\frac{d^2q}{(2\pi)^2},$$

это точный результат, а не приближенный.

Чтобы применить это соотношение в низкоэнергетической области, заметим, что зависимость $F_\varepsilon\left(k_1,k_2\right)$ от k_1 и k_2 имеет характерный масштаб $k_{1,2} \approx a^{-1}$ (??? почему???). Поэтому при малых энергиях $|\varepsilon| \ll \varepsilon_a = \hbar^2/\left(ma^2\right)$ здесь интеграл по q сходится в области, где зависимость F от q несущественна.

$$-\int \frac{F_\varepsilon\left(k_1,q\right)F_\varepsilon\left(q,k_2\right)}{\left(\varepsilon - q^2/2m + i\delta\right)^2}\frac{d^2q}{(2\pi)^2} \approx -\frac{F^2}{4\pi^2}\cdot 2m\int\limits_\varepsilon^{+\infty}\frac{dx}{x^2}$$

$$\frac{\partial}{\partial\varepsilon}F = -\frac{m}{2\pi\hbar^2\varepsilon}F^2.$$

$$F(\varepsilon) = \frac{2\pi\hbar^2}{m\ln\left((\varepsilon+i\delta)/\varepsilon_0\right)},$$

где ε_0 - неизвестная константа. Точка ветвления логарифма при $\varepsilon = 0$ смещена в нижнюю полуплоскость, поскольку вместо ε стоит $\varepsilon + i\delta$. Константа ε_0 вещественна и отрицательна, поскольку при $\varepsilon < 0$ амплитуда F вещественна. Чтобы в этом убедиться, можно записать члены ряда для F, показанные на рис. 3.1, в координатном представлении, где функция Грина имеет вид $G_\varepsilon(r) = -(m/2\pi r)\exp(-\varkappa r)$, $\varkappa^2 = 2m\varepsilon$. Это выражение вещественно при $\varepsilon < 0$. (???)

Если ε_0 находится в низкоэнергетической области, $|\varepsilon_0| \leqslant \varepsilon_a$, то полюс при $\varepsilon = \varepsilon_0$ имеет реальный смысл, и ему соответствует дискретный уровень. В противном случае полюс находится вне области энергий, где применимо сделанное приближение, и поэтому смысла не имеет. Такая ситуация возникает, например, для рассеяния на слабом отталкивающем потенциале, когда ε_0 дается выражением (3.36) с отрицательным U_0.

(?? не, тут не совсем доехал, еще мало понимаю происходящее. плюс 1ю часть дорабатывать нужно про рассеяние, еще не готов к этим темам.)

ЛШ-14 Поляризуемость связанного состояния

Заряженная частица находится в мелкой двумерной яме в основном состоянии. Определим поляризуемость системы в слабом внешнем поле.

а) Используя формализм функции Грина и $F(\varepsilon) = \frac{2\pi\hbar^2}{m\ln((\varepsilon+i\delta)/\varepsilon_0)}$, запишите функцию Грина в импульсном представлении. Сформулируйте правило обхода полюсов, выражающее, что связанное состояние занято, а состояния непрерывного спектра свободны.

б) Выразите дипольный момент системы через точную функцию Грина в импульсном представлении.

в) Рассмотрите поправку к функции Грина, линейную по электрическому полю. Нарисуйте графики, определяющие поляризуемость. Какие из них обращаются в нуль при интегрировании по энергии или импульсам?

Обзор решения

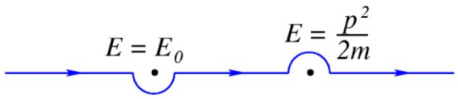
(тут большое решение, потом допишу обзор.)

14.а) определение функции Грина

Согласно формализму функции Грина, $G = G_0 + G_0 F G_0$, где амплитуда $F(\varepsilon) = \frac{2\pi\hbar^2}{m\ln((\varepsilon+i\delta)/\varepsilon_0)}$, что можно получить из дифференцирования диаграмм и решения получившегося уравнения. В импульсном представлении

$$G(\varepsilon, \mathbf{p}, \mathbf{p}') = (2\pi)^2 \frac{\delta^{(2)}(\mathbf{p}-\mathbf{p}')}{\varepsilon - p^2/(2m) + i\delta} + \frac{F(\varepsilon)}{[\varepsilon - p^2/(2m) + i\delta]\,[\varepsilon - p'^2/(2m) + i\delta]}.$$

Положительный знак мнимой части $i\delta$ означает, что состояния непрерывного спектра пусты. При интегрировании по ε эти полюсы надо обходить сверху. Осталось выбрать обход полюса в $F(\varepsilon)$ при $\varepsilon = \varepsilon_0$. Это состояние заполнено, поэтому сдвигаем полюс вверх: $\varepsilon_0 \to \varepsilon_0 + i\delta$. Получаем $F(\varepsilon) = 2\pi\hbar^2/(m\ln(\varepsilon/\varepsilon_0))$, причем обход полюса $\varepsilon = \varepsilon_0$ и точки ветвления $\varepsilon = 0$ такой, как показано на рис. ниже:



14.б) поиск дипольного момента через функцию Грина

$$\begin{aligned}
\mathcal{P} &= e\int \mathbf{r} n(\mathbf{r}) d^2r = -ie\int \lim_{t\to-0} \mathbf{r} G(t,\mathbf{r},\mathbf{r}) d^2r = \\
&= e\iint \left(\int \mathbf{r} e^{i(\mathbf{p}_1-\mathbf{p}_2)\mathbf{r}} d^2r\right)\cdot\left(\lim_{t\to-0}\int e^{-i\omega t} G(\omega,\mathbf{p}_1,\mathbf{p}_2)\frac{d\omega}{2\pi i}\right)\frac{d^2p_1 d^2p_2}{(2\pi)^4} = \\
&= -ie\iint \nabla_1\delta(\mathbf{p}_1-\mathbf{p}_2)\sum \mathrm{Res}_\omega\, G(\omega,\mathbf{p}_1,\mathbf{p}_2)\frac{d^2p_1 d^2p_2}{(2\pi)^2},
\end{aligned}$$

где сумма вычетов берется по всем полюсам ω функции G в верхней полуплоскости ε, что соответствует заполненным уровням. Интегрируя по частям, получаем

$$\mathcal{P} = ie\int \left[\nabla_{\mathbf{p}} \sum \mathrm{Res}_\omega\, G(\omega,\mathbf{p},\mathbf{p}')\right]\Big|_{\mathbf{p}'=\mathbf{p}} \frac{d^2p}{(2\pi)^2}.$$

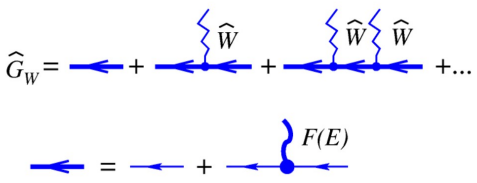
Другую (эквивалентную) форму записи можно получить, если заменить $\nabla_{\mathbf{p}}$ на $\nabla_{\mathbf{p}'}$ и изменить знак.

14.в) Определение поправки и поляризации

Взаимодействие с электрическим полем $W = -eEx$ меняет функцию Грина:

$$\hat{G}_W = \hat{G} + \hat{G}\hat{W}\hat{G} + \hat{G}\hat{W}\hat{W}\hat{G} + \ldots$$

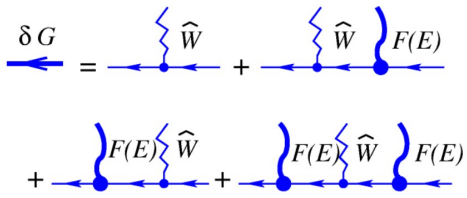
где $\hat{G}$ - точная функция Грина при $E = 0$. Графически это можно представить так:



В импульсном представлении взаимодействию W, линейному по координатам, соответствует производная δ-функции:

$$W(\mathbf{p}) = -\int eEx e^{-i\mathbf{p}\mathbf{r}} d^2r = -ie(2\pi)^2 E\frac{\partial}{\partial p_x}\delta^{(2)}(\mathbf{p}).$$

Для вычисления поляризуемости нужен линейный по полю член ряда (3.45). С учетом структуры G, согласно (3.42), имеем 4 слагаемых (рис. 3.9):



Первое из них есть G_0WG_0. Оно не имеет особенностей над контуром интегрирования по энергии и, поэтому, дает нулевой вклад. Вычислим остальные члены. Выражение $\hat{G}_0W\hat{G}_0\hat{F}\hat{G}_0\,(p,p')$, соответствующее второй диаграмме рис. 3.9, есть:

$$\int \frac{-ieE\partial/\partial p_x\delta^{(2)}\,(\mathbf{p}-\mathbf{p}_1)}{(\varepsilon-p^2/2m+i\delta)}\frac{F(\varepsilon)}{(\varepsilon-p_1^2/2m+i\delta)\,(\varepsilon-p^2/2m+i\delta)}d^2\mathbf{p}_1 =$$
$$= \int \delta\,(\mathbf{p}_1-\mathbf{p})\,\frac{\partial}{\partial p_{1x}}\frac{-ieEF(\varepsilon)}{(\varepsilon-p^2/2m+i\delta)}\times$$
$$\times\frac{1}{(\varepsilon-p_1^2/2m+i\delta)\,(\varepsilon-p^2/2m+i\delta)}d^2\mathbf{p}_1 =$$
$$= -\frac{ieE}{m}F(\varepsilon)\frac{p_x}{(\varepsilon-p^2/2m+i\delta)^3\,(\varepsilon-p^2/2m+i\delta)}.$$

Третье слагаемое получается из второго комплексным сопряжением и перестановкой p и p':

$$\hat{G}_0\hat{F}\hat{G}_0\hat{W}\hat{G}_0\,(\mathbf{p},\mathbf{p}') = \frac{ieEp'_xF(\varepsilon)/m}{(\varepsilon-p^2/2m+i\delta)\,(\varepsilon-p'^2/2m+i\delta)^3}.$$

Последний график $\hat{G}_0\hat{F}\hat{G}_0\hat{W}\hat{G}_0\hat{F}\hat{G}_0\,(p,p')$ равен нулю:

$$ieEF^2(\varepsilon)\iint\frac{d^2p_1d^2p_2}{(2\pi)^2}G_0(\varepsilon,\mathbf{p})G_0\,(\varepsilon,\mathbf{p}_2)\,G_0\,(\varepsilon,\mathbf{p}_1)\,G_0\,(\varepsilon,\mathbf{p}')\,\nabla_{1x}\delta\,(\mathbf{p}_2-\mathbf{p}_1) =$$
$$= -ieEF^2(\varepsilon)G_0(\varepsilon,p)G_0\,(\varepsilon,\mathbf{p}')\int\frac{d^2p_1}{(2\pi)^2}\frac{p_{1,x}/m}{(\varepsilon-p_1^2/2m+i\delta)^3} = 0,$$

как интеграл от нечетной функции. Поэтому

$$\sum_\omega \mathrm{Res}\,G\,(\omega,\mathbf{p},\mathbf{p}') = \mathrm{Res}_{\varepsilon_0}\,F(\varepsilon)\frac{ie}{m}E\left[p'_xG_0\,(\varepsilon_0,\mathbf{p})\,G_0^3\,(\varepsilon_0,\mathbf{p}') - p_xG_0^3\,(\varepsilon_0,\mathbf{p})\,G_0\,(\varepsilon_0,\mathbf{p}')\right].$$

Из-за отмеченной выше симметрии по отношению к перестановке $\mathbf{p}$ и $\mathbf{p}'$ оба слагаемых дают одинаковый вклад в поляризуемость, поскольку и в выражение (3.44) для дипольного момента $\mathcal{P}$ импульсы $\mathbf{p}$ и $\mathbf{p}'$ входят симметрично. Следовательно, достаточно взять только первое слагаемое и удвоить ответ:

$$\mathcal{P}_x = -2\frac{e^2}{m^2}E\int\frac{p_x^2}{(\varepsilon_0-p^2/2m+i\delta)^5}\,\mathrm{Res}_{\varepsilon_0}\,F(\varepsilon)\frac{d^2p}{(2\pi)^2}.$$

Наконец, вычислим поляризуемость

$$\chi_{\alpha\beta} = \frac{2e^2}{m^2}\int\frac{p_\alpha p_\beta(2m)^5}{(p^2+\varkappa^2)^5}\,\mathrm{Res}_{\varepsilon_0}\,F(\varepsilon)\frac{d^2p}{(2\pi)^2},$$

где $\varkappa^2 = 2m|\varepsilon_0|$. Вычислим $\mathrm{Res}_{\varepsilon_0}\,F(\varepsilon)$. Положив $\varepsilon = \varepsilon_0 + z$, разлагаем

$$F(\varepsilon) = \frac{2\pi}{m\ln\,(1+z/\varepsilon_0)} \approx \frac{2\pi\varepsilon_0}{mz}, \qquad \text{откуда} \qquad \mathrm{Res} = \frac{2\pi\varepsilon_0}{m}.$$

Находим

$$\chi_{\alpha\beta} = e^2m^2\varepsilon_0\int\limits_0^{+\infty}\frac{2^6\pi\delta_{\alpha\beta}}{(p^2+\varkappa^2)^5}\frac{p^3dp}{2\pi} = \delta_{\alpha\beta}\frac{16e^2m^2\varepsilon_0}{(2m\varepsilon_0)^3}\int\limits_0^{+\infty}\frac{xdx}{(x+1)^5} = \frac{e^2\delta_{\alpha\beta}}{6m\varepsilon_0^2}.$$

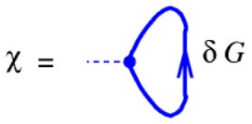
Восстанавливая $\hbar$ по размерности, получаем $\chi = e^2\hbar^2/\left(6m\varepsilon_0^2\right)$.

14.в) Другой способ определения дипольного момента (?????)

К выражению

$$\mathcal{P}_x = -2\frac{e^2}{m^2}E\int \frac{p_x^2}{\left(\varepsilon_0 - p^2/2m + i\delta\right)^5}\,\mathrm{Res}_{\varepsilon_0}\,F(\varepsilon)\frac{d^2p}{(2\pi)^2}.$$

можно прийти несколько быстрее, если заметить, что вершина взаимодействия с электрическим полем устроена точно так же, как и выражение для дипольного момента (3.44). (В координатном представлении (3.50) есть свертка производной δ-функции с функцией Грина по ее аргументам.) Поэтому все вклады в поляризуемость можно представить графически так (рис. 3.10):



Здесь δG дается суммой четырех слагаемых, показанных на рис. 3.9, а штриховая линия обозначает $\nabla\delta(\mathbf{p})$ в импульсном представлении, или $\mathbf{r}$ - в координатном. Первый график на рис. 3.9 дает нуль при интегрировании по энергиям, а четвертый, из-за нечетности $\mathbf{r}$, - обращается в нуль при интегрировании по импульсам. Второй и третий графики отличны от нуля и равны в силу симметрии.

Solution. без диаграмм (????)

(??? можно ли решить эту задачу без диаграмм??? потом попробую. 1D случай для дельта-ямы уже решен.. как этот ответ связан с тем ответом, кстати? пока для меня это два разных значения поляризуемости и всё.)

Пример конкретных мелких 2D ям (????)

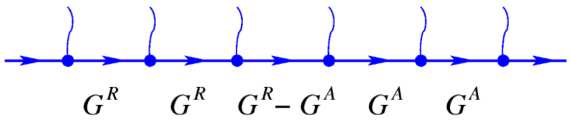
(??? я правильно понимаю, что ε_0 можно запросто определить, зная величину потенциала, а потом подставить сюда???? приведу какой-то пример тут с конкретными значениями!)

ЛШ-15 Теорема унитарности графически

Амплитуда рассеяния $f(\mathbf{k},\mathbf{k}')$ частицы во внешнем поле удовлетворяет теореме унитарности:

$$f(\mathbf{k},\mathbf{k}') - f^*(\mathbf{k}',\mathbf{k}) = \frac{ik}{2\pi}\int f(\mathbf{k},\mathbf{k}'')\,f^*(\mathbf{k}',\mathbf{k}'')\,do''$$

Мы видели, что $F(\mathbf{k},\mathbf{k}') = -\left(2\pi\hbar^2/m\right)f(\mathbf{k},\mathbf{k}')$ дается простой суммой графиков. Поэтому полезно уметь получать соотношение унитарности на графическом языке. Как это сделать? Рассмотрите диаграммы вида

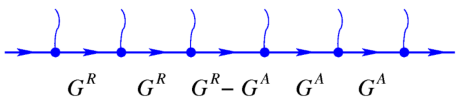


где $G^{R(A)}(\varepsilon,\mathbf{p}) = \frac{1}{\varepsilon - \mathbf{p}^2/2m \pm i\delta}$ — запаздывающая и опережающая функции Грина. Получите левую и правую части равенства теоремы унитарности, просуммировав эти графики двумя разными способами.

Аналогично получите соотношение унитарности в двумерном случае. Какова связь двумерной амплитуды рассеяния $f(\mathbf{k},\mathbf{k}')$ с $F(\mathbf{k},\mathbf{k}')$? Убедитесь, что амплитуда F, найденная в задаче 13, обладает свойством унитарности.

Solution. в 1D

Суммируем диаграммы, изображенные на рис.



С одной стороны, раскрывая по линейности и группируя члены, имеем $F(\mathbf{k},\mathbf{k}')-F^*(\mathbf{k}',\mathbf{k})$, поскольку все остальные члены, содержащие G^R и G^A одновременно, взаимно сокращаются. С другой стороны,

$$G^R-G^A=\frac{1}{\varepsilon-p^2/2m+i\delta}-\frac{1}{\varepsilon-p^2/2m-i\delta}=-2\pi i\delta\left(\varepsilon-p^2/2m\right).$$

И вдобавок, при собирании всех графиков, слева от G^R-G^A возникает выражение $F(\mathbf{k},\mathbf{k}')$, а справа $-F^*(\mathbf{k}',\mathbf{k})$:

$$-2\pi i\int F(\mathbf{k},\mathbf{q})F^*(\mathbf{k}',\mathbf{q})\,\frac{d^3q}{(2\pi)^3}\delta\left(\varepsilon-q^2/2m\right)=-2\pi i\int F(\mathbf{k},\mathbf{q})F^*(\mathbf{k}',\mathbf{q})\,\frac{m}{q}\delta(|\mathbf{q}|-|\mathbf{k}|)do\frac{q^2dq}{(2\pi)^3}=$$
$$=-\frac{imk}{(2\pi)^2}\int F(\mathbf{k},\mathbf{q})F^*(\mathbf{k}',\mathbf{q})\,do.$$

(???? в это пока не въезжаю.)
Сравнивая, получаем теорему унитарности для амплитуды F:

$$F(\mathbf{k},\mathbf{k}')-F^*(\mathbf{k}',\mathbf{k})=-\frac{imk}{(2\pi)^2}\int F(\mathbf{k},\mathbf{q})F^*(\mathbf{k}',\mathbf{q})\,do.$$

Связь с квантовомеханической амплитудой рассеяния, $F=-\left(2\pi\hbar^2/m\right)f$, была найдена в задаче 11.
(??? и какая же она??)
Выражая F через f, приходим к теореме унитарности (3.15).

Solution. в 2D (?)

Повторяя вывод в двумерном случае, получаем

$$F(\mathbf{k},\mathbf{k}')-F^*(\mathbf{k}',\mathbf{k})=-\frac{im}{2\pi}\int F(\mathbf{k},\mathbf{q})F^*(\mathbf{k}',\mathbf{q})\,d\theta$$

В размерности $D=2$ связь F и квантовомеханической амплитуды f другая.
(??? на этом этапе видно, что я вообще не усвоил то, с чем мы работаем.)
Чтобы ее получить, поступим как в задаче 11. Возьмем выражение (3.21) для расходящейся волны, $\chi_{\mathbf{k}}(\mathbf{r})=\langle\mathbf{r}|G_0F|\mathbf{k}\rangle$, верное в любой размерности, и найдем асимптотическое поведение функции G_0:

$$G_0(\varepsilon,\mathbf{r})=\int\frac{e^{i\mathbf{pr}}}{\varepsilon-\hbar^2p^2/2m+i\delta}\frac{d^2p}{(2\pi)^2}\approx-\frac{m}{\hbar^2\sqrt{2\pi k|\mathbf{r}|}}e^{ik|\mathbf{r}|+i\pi/4}$$

при $k|\mathbf{r}|\to\infty$ (см. задачу 6 к §126[2]). Поэтому при $D=2$ амплитуда $f=-\left(m/\hbar^2\sqrt{2\pi k}\right)F$ Поэтому теорема унитарности при $D=2$ гласит:

$$f(\mathbf{k},\mathbf{k}')-f^*(\mathbf{k}',\mathbf{k})=i\sqrt{\frac{k}{2\pi}}\int f(\mathbf{k},\mathbf{q})f^*(\mathbf{k}',\mathbf{q})\,do_q$$

Отметим, что в размерности $D=2$ более удобно включать множитель $e^{i\pi/4}$ в определение расходящейся волны, как это сделано выше, а не в амплитуду рассеяния, как в [2]. При таком определении f, соотношение унитарности принимает наиболее простой вид. Поскольку амплитуда f есть коэффициент при расходящейся волне, включать фазовый множитель в определение f или в выражение для расходящейся волны - дело вкуса.
Воспользуемся случаем, чтобы еще раз отметить существенную разницу между обычной амплитудой f и амплитудой рассеяния в энергетической нормировке F («ужирненной вершиной»). Определение амплитуды F не допускает никакого произвола, поскольку не зависит от выбора выражения для расходящейся волны.

О важности и применимости этой задачи (?????)

Эта задача весьма важна для дальнейшего, поскольку в ней на простейшем примере показан прием, обобщающийся на более сложные случаи. Для любого процесса рассеяния, распада, перехода и т. д. имеется связь между его вероятностью и мнимой частью амплитуды. Эта связь описывается теоремой унитарности. В графическом представлении, мнимая часть какой-либо амплитуды может быть найдена путем разбиения соответствующих диаграмм каким-либо сечением, и заменой функций Грина по одну сторону сечения на комплексно-сопряженные функции. При этом следует просуммировать по всем возможным способам выбора сечения диаграммы. Состояния в сечении имеют смысл конечных состояний распада, рассеяния, и т.п.
(?? не, не знаю, насколько применима она, я не применял, графики - сложно, без них тоже многое решается)

ПТФ.теор Задача Ландау-Зенера методом Лапласа

Задача Ландау - Зенера описывает общий случай «пересечения уровней» (level crossing), и описывается следующим гамильтонианом: $\hat{H} = \begin{pmatrix} \alpha t & \gamma \\ \gamma & -\alpha t \end{pmatrix}$. На $-\infty$ мы имеем волновую функцию $\psi_1 \sim \binom{1}{0}$; Найти вероятность оказаться в каждом из состояний при $t \to \infty$ методом Лапласа.

Напоминание: суть метода Лапласа

(допишу потом)

Solution.

Сводим систему к одному диффуру, делаем преобразование Лапласа, используем метод перевала для двух разных случаев параметра.
(!!!??? решение ниже написано каким-то бездарным человеком, поэтому всё его нужно переписать читабельно. Начать лучше с чтения про эту тему нормальной книги, а не конспекта студентов ПТФ)

$$\begin{cases} i\partial_t \psi_1 = \alpha t \cdot \psi_1 + \gamma \cdot \psi_2 \\ i\partial_t \psi_2 = \gamma \cdot \psi_1 - \alpha t \cdot \psi_2 \end{cases}, \quad |\psi_1(-\infty)|^2 = 1, \quad \psi_2(-\infty) = 0$$

$$z := \alpha^{1/2} t \qquad \beta := \frac{\gamma^2}{2\alpha}$$

$$\psi_1'' + \left(i + 2\beta + z^2\right)\psi_1 = 0$$

$$\psi_1(z) \equiv e^{iz^2/2} f(z)^{17}$$

$$f'' + 2iz \cdot f' + 2(i+\beta) f = 0$$

Применим метод Лапласа:

$$P(t) = t^2 + 2(i+\beta), \qquad Q(t) = 2it, \qquad \int \frac{P}{Q} dt = -\frac{i}{4}t^2 + (-i\beta + 1)\ln t$$

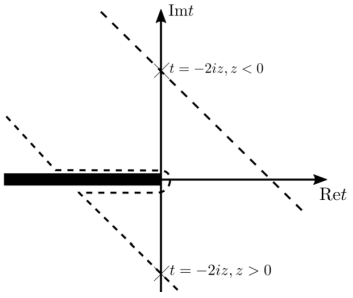
$$f(z) = \int_c dt \cdot t^{-i\beta} \exp\left(-\frac{i}{4}t^2 + zt\right)$$

(?? последнюю формулу нужно прописать, что за формула используется тут??!!!)
Определим седловые точки полученного интеграла:

$$\varphi(t) = -\frac{i}{4}t^2 + zt, \quad \varphi'(t_0) = -\frac{i}{2}t_0 + z = 0 \to t_0 = -2iz, \quad \varphi(t_0) = -iz^2$$

$$\varphi'' = -\frac{i}{2} \to \theta = -\frac{\pi}{4}$$

Таким образом, вклад от седла будет даваться $f(z) \sim e^{-iz^2} \to \psi_1(z) \sim e^{-iz^2/2}$ Кроме этого, для того, чтобы определить многозначную функцию $t^{-i\beta}$, требуется провести разрез.
Вообще говоря, перевальный контур может этот разрез задеть, и в интеграл будет вклад от разреза.



Такой вклад удобно будет оценить, если разрез пустить по вещественной оси влево $t \in (-\infty; 0)$; тогда вдоль разреза функция экспоненциально затухает, и вклад от разреза будет $f \sim 1 \to \psi_1 \sim e^{iz^2/2}$. Исходя

из постановки задачи, мы понимаем, что при $z \to -\infty$ вклад должен быть только от седла, а при $z \to +\infty$ -и от седла, и от разреза.

Это достигается выбором контура, который идёт из 4 четверти во вторую (смотри рисунок).

Случай $z < 0$ Тут имеется только вклад от седла.

При этом многозначная функция $t_0^{-i\beta} = e^{\pi\beta/2} \cdot |t_0|^{-i\beta}$, и получаем (вспоминая, что $\psi_1(z) = e^{-iz^2/2} f(z)\Big)$

$$\psi_1(z \to -\infty) \approx \sqrt{2\pi} e^{\pi\beta/2} e^{-iz^2/2 - i\beta \ln 2|z| - i\pi/4}, \quad |\psi_1(z \to -\infty)|^2 = 2\pi e^{\pi\beta}$$

Воспользуемся первым уравнением, чтобы показать, что $\psi_2(-\infty) = 0$. Подставляя, получаем:

$$\psi_2(z \to -\infty) \approx -\sqrt{\pi\beta} e^{\pi\beta/2} \frac{1}{|z|} e^{-iz^2/2 - i\beta \ln(2|z|) - \frac{i\pi}{4}}, \quad |\psi_2(z \to -\infty)| \approx \frac{\pi\beta e^{\pi\beta}}{z^2} \to 0$$

Тем самым, мы проверили, что найденное решение - ровно то, что мы ищем! Случай $z > 0$ Наша многозначная функция даёт $t_0^{-i\beta} = e^{-\pi\beta/2} |t_0|^{-i\beta}$; тем самым, вклад от седла даётся:

$$\psi_1^{(1)}(z \to +\infty) = \sqrt{2\pi} e^{-\pi\beta/2} e^{-iz^2/2 - i\beta \ln 2z - i\pi/4}, \quad |\psi_1^{(1)}(z \to +\infty)|^2 = 2\pi e^{-\pi\beta/2}$$

Оценим теперь вклад от разреза.

На разных берегах разреза мы имеем:

$$t^{-i\beta} = (-|t|)^{-i\beta} = \begin{cases} e^{\pi\beta} |t|^{-i\beta}, & \operatorname{Im} t = +0 \\ e^{-\pi\beta} |t|^{-i\beta}, & \operatorname{Im} t = -0 \end{cases}$$

Тем самым, вклад от разреза оценивается следующим образом.

На нём затухающая экспонента e^{zt} кважнееэ, чем медленная $e^{-it^2/4}$; получаем:

$$\psi_1^{(2)}(z) = e^{iz^2/2} \left[e^{-\pi\beta} \int\limits_{-\infty}^{0} dt \cdot |t|^{-i\beta} e^{zt} + e^{\pi\beta} \int\limits_{0}^{-\infty} dt |t|^{-i\beta} e^{zt} \right] =$$

$$= e^{iz^2/2} \left(e^{-\pi\beta} - e^{\pi\beta} \right) \int\limits_{0}^{\infty} dt \cdot t^{-i\beta} e^{-zt} = -2 \operatorname{sh} \pi\beta \Gamma(1 - i\beta) \frac{1}{z} e^{i\beta \ln z + iz^2/2},$$

$$|\psi_1^{(2)}(z \to +\infty)|^2 \sim \frac{4\pi\beta \operatorname{sh} \pi\beta}{z^2} \to 0$$

(тут мы воспользовались тем, что $|\Gamma(1 - i\beta)|^2 = \Gamma(1 - i\beta)\Gamma(1 + i\beta) = i\beta \frac{\pi}{\sin(i\pi\beta)} = \frac{\pi\beta}{\operatorname{sh} \pi\beta}\Big)$ Ответ Мы построили все необходимые асимптотики.

Адиабатическое состояние, которое на - ∞ соответствовало в нашем базисе $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, на $+\infty$ соответствует $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Поэтому вероятность адиабатического перехода даётся просто величиной $P = \frac{|\psi_1(t \to +\infty)|^2}{\psi_1(t \to -\infty)|^2} = e^{-2\pi\beta} \equiv e^{-\pi\gamma^2/\alpha}$ (обратим внимание, что вклад от разреза в эту величину, вообще говоря, нулевой). Этот ответ воспроизводит как пертурбативный ответ (при этом $1 - e^{-\pi\gamma^2/\alpha} \approx \pi \frac{\gamma^2}{\alpha}\Big)$, так и адиабатический.

ПТФ-4.y1 Нормировка

Отнормируйте на дельта-функцию от энергии состояния непрерывного спектра, инфинитные в обе стороны для случая потенциала, имеющего различные асимптотики на бесконечностях $U(-\infty) = 0$, $U(+\infty) = U_0$. Для простоты, считайте $E > U_0 > 0$.

Solution.

$$-\frac{\hbar^2}{2m}\psi'' + U(x)\psi = E\psi \to \psi'' + \frac{2m}{\hbar^2}(E - U)\psi = 0$$

$$x \to -\infty \qquad \Rightarrow \qquad \psi'' + \frac{2mE}{\hbar^2}\psi = 0$$

$$\psi(x) = a_L e^{ik_L x} + b_L e^{-ik_L x}, \quad k_L = \frac{\sqrt{2mE}}{\hbar}$$

$$x \to \infty \qquad \Rightarrow \qquad \psi'' + \frac{2m}{\hbar^2}(E - U_0)\psi = 0$$

$$\psi(x) = a_L e^{ik_R x} + b_L e^{-ik_R x}, \quad k_R = \frac{\sqrt{2m(E-U_0)}}{\hbar}$$

$$\psi_k^{(+)}(x) = \begin{cases} e^{ik_L x} + re^{-ik_L x}, & x \to -\infty, \\ te^{ik_R x}, & x \to +\infty, \end{cases} \qquad \psi_k^{(-)}(x) = \begin{cases} t'e^{ik_L x}, & x \to -\infty, \\ e^{ik_R x} + r'e^{-ik_R x}, & x \to +\infty. \end{cases}$$

$$R = |r|^2, \qquad T = \frac{k_R}{k_L}|t|^2, \qquad R + T = 1$$

$$\langle \psi_{k_L}^{(+)} | \psi_{k'_L}^{(+)} \rangle = \int\limits_{-\infty}^{\infty} dx \psi_{k_L}^{(+)*} \psi_{k'_L}^{(+)} = \int\limits_{-\infty}^{\Lambda} dx \psi_{k_L}^{(+)*} \psi_{k'_L}^{(+)} + \int\limits_{\Lambda}^{\infty} dx \psi_{k_L}^{(+)*} \psi_{k'_L}^{(+)} + \int\limits_{-\Lambda}^{\Lambda} dx \psi_{k_L}^{(+)*} \psi_{k'_L}^{(+)}$$

При произвольном значении Λ, последний член конечен при $k = k'$ (а значит и при $E = E'$) и предствляет собой регулярную функцию от k и k'. Поэтому дельта-функциональный вклад возникнуть может только с бесконечности, с первых двух членов. Проводя эти рассуждения для достаточно больших Λ, понимаем, что для нормировки можно пользоваться только асимптотическим представлением волновых функций.

$$\langle \psi_{k_L}^{(+)} | \psi_{k'_L}^{(+)} \rangle = \text{reg.} + \int\limits_{-\infty}^{\Lambda} dx (e^{-ik_L x} + r_k^* e^{ik_L x})(e^{ik'_L x} + r_{k'} e^{-ik'_L x}) + \int\limits_{\Lambda}^{\infty} dx t_k^* e^{-ik_R x} t_{k'} e^{-ik'_R x}$$

Уже в этом выражении заменяя пределы интегрирования на ноль, добавим регулярный вклад, и характер сингулярности не изменится. Поскольку амплитуды являются “медленными огибающими”, то в них мы можем положить $k = k'$.

$$\langle \psi_{k_L}^{(+)} | \psi_{k'_L}^{(+)} \rangle = \text{reg.} + \int\limits_{-\infty}^{0} dx (e^{-i(k_L - k'_L)x} + |r_k|^2 e^{i(k_L - k'_L)x}) + \int\limits_{0}^{\infty} dx |t_k|^2 e^{-i(k_R - k'_R)x}$$

$$k_L^2 - k_L'^2 = \frac{2m(E - E')}{\hbar^2} = k_R^2 - k_R'^2$$

$$k_R - k'_R = \frac{k_R^2 - k_R'^2}{k_R + k'_R} = \frac{k_L^2 - k_L'^2}{k_R + k'_R}$$

$$\int\limits_0^{\infty} dx |t_k|^2 e^{-i(k_R - k'_R)x} = \int\limits_0^{\infty} du \frac{k_R + k'_R}{k_L + k'_L} |t_k|^2 e^{-i(k_L - k'_L)u} = \int\limits_0^{\infty} du \frac{k_R}{k_L} |t_k|^2 e^{-i(k_L - k'_L)u} = \int\limits_0^{\infty} dx T e^{-i(k_L - k'_L)x}$$

$$\langle \psi_{k_L}^{(+)} | \psi_{k'_L}^{(+)} \rangle = \text{reg.} + \int\limits_{-\infty}^{0} dx e^{-i(k_L - k'_L)x} + \int\limits_0^{\infty} R e^{-i(k_L - k'_L)x} + \int\limits_0^{\infty} dx T e^{-i(k_L - k'_L)x} = \int\limits_{-\infty}^{\infty} dx e^{-i(k_L - k'_L)x}$$

$$\langle \psi_{k_L}^{(+)} | \psi_{k'_L}^{(+)} \rangle = \text{reg.} + 2\pi\delta(k_L - k'_L) = \text{reg.} + \frac{2\pi\hbar}{\sqrt{2m}} \delta(\sqrt{E} - \sqrt{E'}) = \text{reg.} + \frac{2\pi\hbar}{\sqrt{2m}} \delta\left(\frac{E - E'}{\sqrt{E} + \sqrt{E'}} \right)$$

$$\langle \psi_E^{(+)} | \psi_{E'}^{(+)} \rangle = \text{reg.} + 2\pi\hbar \sqrt{\frac{2E}{m}} \delta(E - E')$$

ПТФ-4.y2 Полнота состояний в дельта-потенциале

Рассмотрите движение одномерной частицы в поле мелкой ямы, $U(x) = -\frac{\kappa}{m}\delta(x)$. Покажите непосредственным вычислением полноту базиса собственных состояний гамильтониана. Рассмотрите как случай $\kappa > 0$ (когда в яме имеется связанное состояние), так и $\kappa < 0$.

Указание: при проверке условия полноты, $\delta(x - x') = \sum\limits_n \psi_n^*(x)\psi_n(x')$, для простоты можете рассмотреть только случай $x, x' > 0$.

Solution.

(!!! важно дописать основную идею, пока не думал много про это??!!)

$$\psi_k^{(+)}(x) = \begin{cases} e^{ikx} + re^{-ikx}, & x \to -\infty \\ te^{ikx}, & x \to +\infty \end{cases} \quad , \quad \psi_k^{(-)}(x) = \begin{cases} t'e^{ikx}, & x \to -\infty \\ e^{ikx} + r'e^{-ikx}, & x \to +\infty \end{cases}$$

Граничные условия дают:

$$1 + r = t, \qquad ikt - (ik - ikr) = -2\kappa t \qquad \to \qquad t = \frac{ik}{\kappa + ik}, \qquad r = \frac{\kappa}{\kappa + ik}$$

$$t' = t, \qquad r' = -\frac{r^*}{t^*}t = \frac{\kappa}{ik}\frac{-ik}{\kappa + ik} = -\frac{\kappa}{\kappa + ik} = r$$

(???? непонятно, откуда выражение ниже?)

$$f(x, x') = \frac{1}{2\pi}\int\limits_0^\infty dk(e^{ik(x-x')} + |r|^2 e^{-ik(x-x')} + |t|^2 e^{-ik(x-x')} + re^{ik(x+x')} + r^* e^{-ik(x+x')}) =$$

$$= \frac{1}{2\pi}\int\limits_0^\infty dk(e^{ik(x-x')} + e^{-ik(x-x')}) + \frac{1}{2\pi}\int\limits_0^\infty dk\left(\frac{\kappa}{\kappa + ik}e^{ik(x+x')} + \frac{1}{2\pi}\frac{\kappa}{\kappa - ik}e^{-ik(x+x')}\right)$$

$$\int\limits_0^\infty dk(e^{ik(x-x')} + e^{-ik(x-x')}) = \int\limits_{-\infty}^\infty dke^{ik(x-x')} = 2\pi\delta(x - x')$$

$$\int\limits_0^\infty dk\left(\frac{\kappa}{\kappa + ik}e^{ik(x+x')} + \frac{\kappa}{\kappa - ik}e^{-ik(x+x')}\right) = \int\limits_{-\infty}^\infty dk\frac{\kappa}{\kappa + ik}e^{ik(x+x')} \overset{\text{res}}{=} \begin{cases} 2\pi\exp(-\kappa(x + x')), & \kappa > 0 \\ 0, & \kappa < 0 \end{cases}$$

For $\kappa < 0$:

$$f(x, x') = \delta(x - x')$$

For $\kappa > 0$: Добавим к $f(x, x')$ связанное состояние $\psi_0(x)$: $\psi_0^*(x)\psi_0(x') = \kappa e^{-\kappa(|x|+|x'|)}$. Тогда и в этом случае

$$f(x, x') = \delta(x - x')$$

Таким образом, соотношение полноты доказано в обоих случаях.

Давнее вроде неверное решение

Требуется для потенциала вида "ступеньки" отнормировать на δ-функцию состояния непрерывного спектра, то есть найти $c(f)$ в выражении

$$\langle\psi_f|\psi_{f'}\rangle = c(f)\delta\left(f - f'\right)$$

Обозначим $k = \sqrt{2mE}, k' = \sqrt{2m\left(E - U_0\right)}$,
решения УШ имеют вид

$$\Psi_k^+(x) = \begin{cases} e^{ikx} + r(k)e^{-ikx}, & x \longrightarrow -\infty \\ t(k)e^{ik'x}, & x \longrightarrow +\infty \end{cases} .$$

из непрерывности получаем коэффициенты

$$1 + r = t, \quad k(1 - r) = k'r; \quad r(k) = \frac{k - k'}{k + k'}, \quad t(k) = \frac{2k}{k + k'}$$

переписав скалярное произведение подобно тому, как сделано на семинаре:

$$\int\limits_{-\infty}^\infty dx\psi_{f'}^*(x)\psi_f(x) = \int\limits_{-\infty}^{-\lambda} dx\psi_{f'}^*(x)\psi_f(x) + \int\limits_{\lambda}^\infty dx\psi_{f'}^*(x)\psi_f(x) + \int\limits_{-\lambda}^{\lambda} \psi_{f'}^*(x)\psi_f(x)dx$$

придем к

$$\langle\psi_k|\psi_{k'}\rangle = \text{reg}\,. + \int\limits_{-\infty}^{-\lambda} \left(e^{-ikx} + r_k^* e^{ikx}\right)\left(e^{ik'x} + r_{k'}e^{-ik'x}\right)dx + \int\limits_{\lambda}^{\infty} t_k^* e^{-ikx} t_{k'} e^{ik'x} dx$$

и мб я не до конца понимаю что-то, но у нас вроде бы все то же, что в случае

$$\langle\psi_k|\psi_{k'}\rangle = \text{reg} + \int\limits_{-\infty}^{\infty} e^{-i\left(k-k'\right)x} dx = 2\pi\delta\left(k-k'\right)$$

в итоге нормировка такая:

$$\langle\psi_k|\psi_{k'}\rangle = \text{reg} + \int\limits_{-\infty}^{\infty} e^{-i\left(k-k'\right)x} dx = 2\pi\delta\left(k-k'\right)$$

ПТФ-4.з1. Выключение и включение потенциала

1. Частица находится в основном состоянии гармонического осциллятора $U(x) = \frac{m\omega^2 x^2}{2}$. Потенциал выключают на время T, спустя которое его снова включают. Определите вероятность того, что частица окажется в *основном* состоянии.

2. Этот же вопрос, но для $-\frac{\hbar^2\kappa}{m}\delta(x)$ и для случаев малых и больших времён T.

Подсказка: для асимптотической оценки интеграла в пункте 2 для случая малых T вам может пригодиться приём – преобразование Хаббарда-Стратановича (преобразующее экспоненту от квадратом A в выражение экспонентой от просто A):

$$e^{-iA^2} = \frac{e^{\frac{i\pi}{4}}}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} dz e^{iz^2 - 2izA}$$

Solution. в общем случае

$$-\frac{\hbar^2}{2m}\psi'' + U(x)\psi = E\psi \to \psi'' + \frac{2m}{\hbar^2}\left(E - U(x)\right)\psi = 0$$

$$\Psi(p) = \int\limits_{-\infty}^{\infty} \psi(x) \exp\left(-\frac{ipx}{\hbar}\right) dx$$

$U = 0 \Rightarrow$

$$i\hbar\frac{\partial\Psi(p,t)}{\partial t} = \langle p|\hat{H}(t)|\psi(t)\rangle = \frac{p^2}{2m}\Psi(p,t), \quad \Psi(p,0) = \Psi(p)$$

$$\Psi(p,T) = \Psi(p)\exp\left(-\frac{ip^2}{2m\hbar}T\right)$$

$$P_{\text{gr}\to\text{ gr}} = \left|\int\limits_{-\infty}^{\infty} (dp)\Psi^*(p)\Psi(p,T)\right|^2 = \left|\int\limits_{-\infty}^{\infty} (dp)\Psi^2(p)\exp\left(-\frac{ip^2}{2m\hbar}T\right)\right|^2$$

Solution. для гармонического осциллятора

$$U(x) = \frac{m\omega^2 x^2}{2}$$

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

$$\Psi(p) = \int\limits_{-\infty}^{\infty} \psi(x)\exp\left(-\frac{ipx}{\hbar}\right)dx = \sqrt{2}\left(\frac{\pi\hbar}{m\omega^3}\right)^{\frac{1}{4}} \exp\left(-\frac{p^2}{2m\omega^2\hbar}\right)$$

$$\Psi_{U=0}(p,T)=\Psi(p)\exp\left(-\frac{ip^2}{2m\hbar}T\right)$$

$$\begin{aligned}P_{\text{gr}\to\text{ gr}}(T)&=\left|\int\limits_{-\infty}^{\infty}(dp)\Psi^2(p)\exp\left(-\frac{ip^2}{2m\hbar}T\right)\right|^2=\\&=\left|\int\limits_{-\infty}^{\infty}(dp)\left(\sqrt{2}\left(\frac{\pi\hbar}{m\omega^3}\right)^{\frac{1}{4}}\exp\left(-\frac{p^2}{2m\omega^2\hbar}\right)\right)^2\exp\left(-\frac{ip^2}{2m\hbar}T\right)\right|^2=\\&=\frac{1}{\sqrt{1+\frac{\omega^2T^2}{4}}}\end{aligned}$$

Solution. для дельта-потенциала

$$U(x)=-\frac{\hbar^2\kappa}{m}\delta(x)$$

$$\psi(x)=\sqrt{\kappa}\exp(-\kappa|x|)$$

$$\Psi(p)=\int\limits_{-\infty}^{\infty}\psi(x)\exp\left(-\frac{ipx}{\hbar}\right)dx=\frac{2\kappa^{\frac{3}{2}}\hbar^2}{p^2+\kappa^2\hbar^2}$$

Вероятность того, что частица окажется в основном состоянии:

$$P_{\text{gr}\to\text{ gr}}(T)=\left|\int\limits_{-\infty}^{\infty}(dp)\Psi^2(p)\exp\left(-\frac{ip^2}{2m\hbar}T\right)\right|^2=\left|\int\limits_{-\infty}^{\infty}(dp)\left(\frac{2\kappa^{\frac{3}{2}}\hbar^2}{p^2+\kappa^2\hbar^2}\right)^2\exp\left(-\frac{ip^2}{2m\hbar}T\right)\right|^2$$

$A:=p\sqrt{\frac{T}{2m\hbar}}$,

$$e^{-iA^2}=\frac{e^{\frac{i\pi}{4}}}{\sqrt{\pi}}\int\limits_{-\infty}^{\infty}dze^{iz^2-2izA}=\frac{e^{\frac{i\pi}{4}}}{\sqrt{\pi}}\int\limits_{-\infty}^{\infty}dze^{iz^2-2izp\sqrt{\frac{T}{2m\hbar}}}$$

$$P(T)=\left|\int\limits_{-\infty}^{\infty}(dp)\left(\frac{2\kappa^{\frac{3}{2}}\hbar^2}{p^2+\kappa^2\hbar^2}\right)^2\frac{e^{\frac{i\pi}{4}}}{\sqrt{\pi}}\int\limits_{-\infty}^{\infty}dze^{iz^2-2izp\sqrt{\frac{T}{2m\hbar}}}\right|^2$$

Проинтегрируем по p при помощи вычетов (полюсы в $p=\pm i\kappa\hbar$ второго порядка):

(так вроде и получается, еще раз на бумажке проделаю. Пока не досмотрел, вычеты 2го порядка, так ли они получаются как написано?)

$$\begin{aligned}P(T)&=\frac{16\kappa^6\hbar^8}{4\pi^3\hbar^2}\frac{\pi^2}{4\hbar^6\kappa^6}\left|2\int\limits_0^{\infty}dze^{-2\kappa\hbar\sqrt{\frac{T}{2m\hbar}}z}\left(1+2\kappa\hbar\sqrt{\frac{T}{2m\hbar}}z\right)e^{iz^2}\right|^2\\&=\frac{4}{\pi}\left|\int\limits_0^{\infty}dze^{-\kappa\sqrt{\frac{2\hbar T}{m}}z}\left(1+\kappa\sqrt{\frac{2\hbar T}{m}}z\right)e^{iz^2}\right|^2\\&=\frac{4}{\pi}\left|\frac{1}{8}\left(4ia+(1+i)(a^2+2i)e^{i\frac{a^2}{4}}\sqrt{2}\pi(-i-(1-i)\int\limits_0^{a/\sqrt{2}\pi}dt\cos^2t+(1+i)\int\limits_0^{a/\sqrt{2}\pi}dt\sin^2t\right)\right|^2\end{aligned}$$

(????? последний переход нужно сидеть и продумывать. во-первых там скобка пропущена. во-вторых, вообще пока не вижу, как его получили, тут много шагов упущено, нужно вписать их!)

$$\int\limits_0^{a/\sqrt{2}\pi}dt\cos^2t\sim x,\qquad\int\limits_0^{a/\sqrt{2}\pi}dt\sin^2t\sim\frac{x^3}{3}$$

(?? это ужасное решение, нужно переписать, x тут не определен, нужно продумывать с начала)
$a := \sqrt{\frac{2\hbar T}{m}}\kappa \ll 1$,

$$P(T) = \frac{4}{\pi}\left|\frac{1+i}{2}\sqrt{\frac{\pi}{2}} + \frac{\sqrt{\pi}(1-i)}{8\sqrt{2}}a^2 + \mathcal{O}(a^3)\right|^2 = \frac{4}{\pi}\left(\frac{\pi}{4} - \frac{\sqrt{\pi}}{6\sqrt{2}}a^3\right) = 1 - \frac{4\sqrt{\pi}}{6\sqrt{2}\pi}a^3 + \mathcal{O}(a^3)$$

При малых временах T:

$$P(T) = 1 - \frac{4\kappa^3}{3\sqrt{\pi}}\left(\frac{\hbar T}{m}\right)^{\frac{3}{2}} + \mathcal{O}(T^3)$$

При больших временах T: $\int\limits_0^{a/\sqrt{2}\pi} dt \cos^2 t \sim \sqrt{\frac{\pi}{8}} - \frac{\cos x^2}{2x}$, $\int\limits_0^{a/\sqrt{2}\pi} dt \sin^2 t \sim \sqrt{\frac{\pi}{8}} + \frac{\sin x^2}{2x}$,

$$P(T) = \frac{4}{\pi}\left|\frac{2}{a} + \mathcal{O}\left(\frac{1}{a^3}\right)\right| = \frac{16}{\pi a^2} + \mathcal{O}\left(\frac{1}{a^3}\right) = \frac{8m}{\pi\hbar\kappa^2 T} + \mathcal{O}\left(\frac{1}{T^3}\right)$$

Solution. еще одно, давнее

Определим основные состояния при включенном потенциале, то есть решим стационарное УШ:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + \frac{m\omega^2 x^2}{2}\psi(x) = E\psi(x)$$

связное состояние имеет вид:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \cdot \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

После выключения потенциала эволюция системы будет описываться УШ:

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi \quad \hat{H} = \frac{\hat{p}^2}{2m}$$

собственные значения энергии: $\frac{p^2}{2m}\varphi = \lambda\varphi$, по итогу эволюция волновой функции происходит: $\hat{U}(t) = e^{-i(p^2/(2m\hbar))T}$

Так как тут имеется только оператор импульса, то представим волновую функцию в импульсном представлении, дальше

$$\psi(p) = \int dx e^{-ipx/\hbar}\psi(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\int dx e^{-ipx/\hbar}\cdot e^{\left(-\frac{m\omega x^2}{2\hbar}\right)}$$

(? какие-то преобразования)
и приходим к

$$\psi(p) = \left(\frac{4\pi\hbar}{m\omega}\right)^{1/4}\exp[-p^2/(2m\omega\hbar)]$$

таким образом, эволюция происходит так:

$$\psi_p(T) = \left(\frac{4\pi\hbar}{m\omega}\right)^{1/4}\exp[-p^2/(2m\omega\hbar)]e^{-i(p^2/(2m\hbar))T}$$

$$\psi_x(T) = \frac{1}{2\pi\hbar}\int\limits_{-\infty}^{\infty}\left(\frac{4\pi\hbar}{m\omega}\right)^{1/4}\exp[-p^2/(2m\omega\hbar)]e^{-i(p^2/(2m\hbar))T}e^{ipx/\hbar}$$

Вероятность нахождения опять в основном состоянии определяется ($\hbar = 1$)

$$A = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\left(\frac{4\pi\hbar}{m\omega}\right)^{1/4}\exp[-p^2/(2m\omega\hbar)]e^{-i(p^2/(2m\hbar))T}e^{ipx/\hbar}e^{-\kappa|x|}dxdk$$

(??)

Solution. еще одно, давнее

для потенциала $U(x) = -\frac{\kappa}{m}\delta(x)$ решение имеет вид:

$$\psi(x) = \sqrt{\kappa}e^{-\kappa|x|}$$

После отключения потенциала данная волновая функция начнет эволюционировать, а так как она представляется в виде разложения по базису из континуума волн - по спектру оператора импульса, то в импульсном представлении мы знаем, как будет каждая компонента эволюционировать.
(здесь и далее $p \equiv k$)

$$\psi(k) = \int\limits_{-\infty}^{\infty} \psi(x)e^{-ikx}dx = \sqrt{\kappa}\int\limits_{-\infty}^{\infty} e^{-\kappa|x|-ikx}dx \overset{wolfram}{=} \frac{2\kappa^{\frac{3}{2}}}{\kappa^2+k^2}$$

вспоминая $\hat{U}(t) \equiv \exp(-i\hat{H}t/\hbar)$, получаем оператор эволюции ($p \equiv k$):

$$\hat{U}(t) = e^{-i\frac{k^2}{2m}T}$$

Обратно, в координатном представлении эволюция волновой функции происходит так:

$$\psi(x,T) = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty} \frac{2\kappa^{\frac{3}{2}}}{\kappa^2+k^2}e^{-i\frac{k^2}{2m}T}e^{ikx}dk$$

Вероятность прийти в стационарное состояние через время T - проекция на волновую функцию этого состояния:

$$A = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} \frac{2\kappa^2}{\kappa^2+k^2}e^{-i\frac{k^2}{2m}T}e^{ikx}e^{-\kappa|x|}dxdk$$

Остается привести к понятному виду:

$$A = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty} \frac{2\kappa^2}{\kappa^2+k^2}e^{-i\frac{k^2}{2m}T}\left[\int\limits_{-\infty}^{\infty} e^{ikx}e^{-\kappa|x|}dx\right] = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty} \frac{4\kappa^3}{\left(\kappa^2+k^2\right)^2}e^{-i\frac{k^2}{2m}T}dk$$

Воспользуемся преобразованием Хаббарда-Стратоновича $e^{-iA^2} = \frac{e^{i\pi/4}}{\sqrt{\pi}}\int\limits_{-\infty}^{\infty} dze^{iz^2-2izA}$:

$$A = \frac{e^{i\pi/4}}{\sqrt{\pi}}\frac{1}{2\pi}\int\limits_{-\infty}^{\infty} \frac{4\kappa^3}{\left(\kappa^2+k^2\right)^2}dk\int\limits_{-\infty}^{\infty} dze^{iz^2-2iz\sqrt{\frac{T}{2m}}k} = \frac{-1}{\sqrt{\pi}}e^{i\pi/4}\int\limits_{-\infty}^{\infty} dze^{iz^2-2\kappa\sqrt{\frac{T}{2m}}z}(1+2\kappa\sqrt{\frac{T}{2m}}z)$$

теперь посчитаем то, к чему мы пришли, $c \equiv \sqrt{\frac{2T\kappa^2}{m}}$:

$$\boxed{A = \frac{-e^{i\pi/4}}{\sqrt{\pi}}\int\limits_{-\infty}^{\infty} e^{iz^2-c|z|}(1+c|z|)dz = \frac{-2e^{i\pi/4}}{\sqrt{\pi}}\int\limits_{0}^{\infty} e^{iz^2-cz}(1+cz)dz}$$

для $T \ll 1$
Сделаем замену $z = e^{i\pi/4}x$.
Тогда $a = \frac{-2i}{\sqrt{\pi}}\int\limits_0^{\infty} e^{-x^2-ce^{i\pi/4}x}\left(1+ce^{i\pi/4}x\right)dx$

$$e^{-x^2-ce^{i\pi/4}x} \simeq e^{-x^2}\left(1-ce^{i\pi/4}x+\frac{ic^2x^2}{2}\right)$$

$$e^{-ce^{i\pi/4}x}\left(1+ce^{i\pi/4}x\right) \simeq 1-\frac{ic^2x^2}{2}+\frac{c^3x^3e^{3i\pi/4}}{3}$$

$$a = \frac{-2i}{\sqrt{\pi}}\int\limits_0^{\infty} e^{-x^2}\left[1-\frac{ic^2x^2}{2}+\frac{c^3x^3e^{3i\pi/4}}{3}\right] = -i\left[1-\frac{ic^2}{4}+\frac{c^3(i-1)}{3\sqrt{2\pi}}\right]$$

Для $T \gg 1$ так и хочется применить метод стационарной фазы или метод перевала, но я за 40 мин не разобрался как, так что

ПТФ-4.з2.1. Распад квазистационарного состояния

В этой задаче мы будем исследовать уравнение Шрёдингера в потенциале следующего вида:

$$U(x) = \begin{cases} \infty, & x < 0 \\ \frac{\kappa}{m}\delta(x-a), & x > 0 \end{cases}$$

Рассеивающий потенциал (величину κ) мы будем предполагать сильным. Если заменить этот потенциал на бесконечную стенку, то в этой задаче имеется множество стационарных состояний вида $\psi_n(x) = \sin knx$, $k_n = \frac{\pi n}{a}$ и $E_n^{(0)} = \frac{k_n^2}{2m}$. Возможность туннелирования превращает эти состояния в *квазистационарные* – хоть и не стационарные, но долгоживущие, и на достаточно небольших промежутках времени их можно считать стационарными. Ниже будут изложены три различных точки зрения на такие состояния и показана их эквивалентность.

Указание: хоть дальше и идёт речь об энергетическом представлении – во всех промежуточных вычислениях удобнее пользоваться квантовым числом — импульсом $k = \sqrt{2mE}$.

В начальный момент времени частица была «приготовлена» в одном из квазистационарных состояний, $\psi(x, t = 0) = \psi_0(x)\sqrt{\frac{2}{a}}\sin k_n x$.

• Определите непрерывный спектр исходной задачи, нормированный на дельта-функцию от разницы энергий.

• Рассмотрите разложение исходной волновой функции по этому непрерывному спектру. Обратите внимание, что $|\psi(E)|^2$ вблизи $E_n^{(0)}$ имеет максимум; покажите, что в окрестности этого максимума вероятность устроена как лоренциан:

$$|\psi(E)|^2 \approx c\frac{\Gamma_n}{(E-E_n)^2 + \frac{\Gamma_n^2}{4}}$$

и при этом E_n близка к $E_n^{(0)}$, а $\Gamma_n \ll E_n$. Найдите величины c, E_n, Γ_n.

• Найдите амплитуду того, что через достаточно большое время t частица останется в в этом квазистационарном состоянии $c(t) = \int \psi_0^*(x)\psi(x,t)dx$. Покажите, что на достаточно больших временах соответствующая вероятность $P(t) = |c(t)|^2$ затухает экспоненциально $P(t) \propto \exp(-t/\tau)$. Определите соответствующее «время жизни» τ_n.

Найденное “время жизни” окажется достаточно большим. Это означает, что на временах $t \ll \tau_n$, состояние $|n\rangle$ практически стационарно – волновая функция не меняется, за исключением тривиальной динамической фазы $e^{-iE_n t}$.

Solution.

$$|\psi(E)|^2 = \frac{1}{8\sqrt{2mE}\pi k_n}\frac{\frac{k_n^3}{2m\kappa^2 a}}{(E - E_n^{(0)}(1-\frac{1}{2\kappa a}))^2 + \frac{1}{4}(\frac{k_n^3}{2m\kappa^2 a})^2}$$

$$c = \frac{1}{8\sqrt{2mE}\pi k_n}, \quad E_n = E_n^{(0)}\left(1 - \frac{1}{2\kappa a}\right), \quad \Gamma_n = \frac{k_n^3}{2m\kappa^2 a}$$

Как видно, E_n близко к $E_n^{(0)}$ и $\Gamma_n \ll E_n$.

$$\psi(E) = \sqrt{c}\frac{\sqrt{\Gamma_n}}{(E-E_n) + \frac{i\Gamma_n}{2}}$$

ПТФ-4.з2.2. Задержка волнового пакета

Другой способ смотреть на квазистационарные состояния – это исследовать задачу рассеяния.

• Определите волновые функции исходной задачи, которые соответствуют задаче рассеяния, то есть имеющие асимптотическое поведение $\psi(x \to \infty) = e^{-ikx} + re^{ikx}$. Величина коэффициента отражения $R = |r|^2$ тривиальным образом равна единице, поскольку движение инфинитно только в одну сторону; но вот амплитуда отражения $r(E) \equiv e^{i\delta(E)}$ имеет нетривиальные свойства.

• Покажите, что амплитуда r, как функция *комплексной* энергии ε имеет серию полюсов, близких к вещественной оси $\varepsilon_n = E_n - \frac{i\Gamma_n}{2}$. Покажите, что на вещественной оси в окрестности $E \approx E_n$ амплитуда устроена следующим образом:

$$r(E) \approx e^{i\phi}\frac{E - E_n - \frac{i\Gamma_n}{2}}{E - E_n + \frac{i\Gamma_n}{2}}$$

(с такими же величинами E_n и Γ_n; такой вид связан с условием $|r|^2 = 1$). Как при этом устроена фаза рассеяния $\delta(E)$?

• Рассмотрите нестационарную задачу рассеяния: пусть на такую систему налетает волновой пакет, локализованный по энергии вблизи одного из таких метастабильных состояний, $E \approx E_n$. Определите время задержки такого волнового пакета $\tau = \hbar\frac{\partial\delta}{\partial E}$; и покажите, что непосредственно при резонансе $E = E_n$, время задержки связано с временем жизни метастабильного состояния. Обратите внимание – существенно, что полюса находятся в нижней комплексной полуплоскости; в противном случае мы бы получили $\tau(E_n) < 0$, что очевидным образом противоречит причинности.

С этим эффектом связана иная физическая интерпретация квазистационарных состояний: при рассеянии на резонансе частица «попадает» в метастабильное состояние, где она «застревает» на достаточно продолжительное время, и лишь затем вылетает.

Solution.

•
$$\psi(x \to \infty) = e^{-ikx} + re^{ikx}$$

• Амплитуда отражения:

$$r = \frac{1 - \frac{i\kappa}{k}(1 - e^{-2ika})}{-1 - \frac{i\kappa}{k}(1 - e^{2ika})} = -e^{-2ika}\frac{ke^{ika} - i\kappa e^{ika} + i\kappa e^{-ika}}{ke^{-ika} + i\kappa e^{-ika} - i\kappa e^{ika}} =$$

$$= e^{-2i(k-k_n)a}\frac{ik_n(k-k_n)a + k_n + 2\kappa(k-k_n)a}{ik_n(k-k_n)a - k_n - 2\kappa(k-k_n)a}$$

$$k_n(k-k_n) = \frac{m(E - E_n^{(0)})}{\hbar^2}$$

$$r = e^{-2i(k-k_n)a}\frac{ia\frac{m(E-E_n^{(0)})}{\hbar^2} + k_n + 2\kappa a\frac{m(E-E_n^{(0)})}{k_n\hbar^2}}{ia\frac{m(E-E_n^{(0)})}{\hbar^2} - k_n - 2\kappa a\frac{m(E-E_n^{(0)})}{k_n\hbar^2}}$$

Полюсы:

$$i(E - E_n^{(0)}) - \frac{\hbar^2 k_n}{ma} - \frac{2\kappa}{k_n}(E - E_n^{(0)}) = 0$$

$$(E - E_n^{(0)})\left(i - \frac{2\kappa}{k_n}\right) = \frac{\hbar^2 k_n}{ma}$$

$$E - E_n^{(0)} = \frac{\hbar^2 k_n^2}{2\kappa ma}\frac{1}{\frac{ik_n}{2\kappa} - 1} \approx -\frac{\hbar^2 k_n^2}{2\kappa ma}\left(1 + \frac{ik_n}{2\kappa}\right) = -\frac{\hbar^2 E_n^{(0)}}{\kappa a} - \frac{i\hbar^2 k_n^3}{4\kappa^2 ma}$$

$$E_n = E_n^{(0)}\left(1 - \frac{\hbar^2}{\kappa a}\right) - \frac{i\hbar^2 k_n^3}{4\kappa^2 ma}$$

$$r = \frac{E - E_n - i\frac{\Gamma_n}{2}}{E - E_n + i\frac{\Gamma_n}{2}} = \frac{(E - E_n - i\frac{\Gamma_n}{2})^2}{(E - E_n)^2 + \frac{\Gamma_n^2}{4}} = \frac{(E - E_n)^2 - \frac{\Gamma_n^2}{4} - i\Gamma_n(E - E_n)}{(E - E_n)^2 + \frac{\Gamma_n^2}{4}}$$

$$\delta(E) = -\arctan\frac{\Gamma_n(E - E_n)}{(E - E_n)^2 - \frac{\Gamma_n^2}{4}}$$

• Время задержки:

$$\tau(E) = \hbar\frac{\partial\delta}{\partial E} = \frac{\Gamma_n\hbar}{(E - E_n)^2 + \frac{\Gamma_n^2}{4}}$$

$$\tau(E_n) = \frac{4\hbar}{\Gamma_n}$$

ПТФ-13.y2. Соотношение унитарности

Исходя из соотношения унитарности на языке T-матрицы,

$$\hat{T}_E - \hat{T}_E^\dagger = -2\pi i\hat{T}_E^\dagger\delta(E - \hat{H}_0)\hat{T}_E$$

получите соотношение унитарности на языке амплитуды рассеяния:

$$f(\mathbf{n}, \mathbf{n}') - f^*(\mathbf{n}', \mathbf{n}) = i\frac{k}{2\pi}\int d\mathbf{n}'' f(\mathbf{n}, \mathbf{n}'')f^*(\mathbf{n}', \mathbf{n}'')$$

Solution.

Связь T-матрицы и амплитуды рассеяния:

$$f(\mathbf{n},\mathbf{n}') = -\frac{m}{2\pi}\langle \mathbf{k}'|\hat{T}_E|\mathbf{k}\rangle$$

$$f(\mathbf{n},\mathbf{n}') - f^*(\mathbf{n}',\mathbf{n}) = -\frac{m}{2\pi}(\langle \mathbf{k}'|\hat{T}_E|\mathbf{k}\rangle - \langle \mathbf{k}'|\hat{T}_E^\dagger|\mathbf{k}\rangle) = -\frac{m}{2\pi}\langle \mathbf{k}'|(\hat{T}_E - \hat{T}_E^\dagger)|\mathbf{k}\rangle \quad = im\langle \mathbf{k}'|\hat{T}_E^\dagger\delta(E-\hat{H}_0)\hat{T}_E|\mathbf{k}\rangle =$$
$$= im\int \frac{d^3\mathbf{q}}{(2\pi)^3}\langle \mathbf{k}'|\hat{T}_E^\dagger|\mathbf{q}\rangle\langle \mathbf{q}|\hat{T}_E|\mathbf{k}\rangle\delta(E-E_{\mathbf{q}})$$

$$E = \frac{k^2}{2m} \qquad \Rightarrow \qquad \delta(E-E_{\mathbf{q}}) = \frac{m}{k}\delta(k-|\mathbf{q}|)$$

$$f(\mathbf{n},\mathbf{n}') - f^*(\mathbf{n}',\mathbf{n}) = im\frac{4\pi^2}{(2\pi)^3m^2}\frac{m}{k}k^2\int d\mathbf{n}''f(\mathbf{n},\mathbf{n}'')f^*(\mathbf{n}',\mathbf{n}'') = \frac{ik}{2\pi}\int d\mathbf{n}''f(\mathbf{n},\mathbf{n}'')f^*(\mathbf{n}',\mathbf{n}'')$$

ПТФ-13.з1. Функции Грина и Борновское приближение в 1D и 2D

Одномерие. Выведите формулы Борновского приближения для одномерного пространства. Амплитуда рассеяния определяется согласно:

$$\psi(\mathbf{r}) = e^{i\mathbf{kr}} + f(\mathbf{n},\mathbf{n}')ie^{ik|\mathbf{r}|}$$

Что из себя представляет величина f и как она связана с амплитудами прохождения и отражения t, r? Что из себя представляет сечение рассеяния в одномерии?

Двумерие. Повторите вывод для двумерного пространства. В двумерии амплитуда определяется согласно:

$$\psi(\mathbf{r}) = e^{i\mathbf{kr}} + f(\mathbf{n},\mathbf{n}')e^{\frac{i\pi}{4}}\frac{e^{ikr}}{\sqrt{r}}$$

Указание: функция Грина свободного движения выражается через какие-то из модифицированных функций Бесселя.

Solution. в общем случае

Задача полностью по теории, однако, это очень непростые переходы и задача стоящая.

Пусть $\hat{H}_0 := \frac{\hat{p}^2}{2m}$; $|\mathbf{k}\rangle$ – падающая плоская волна, $|\chi\rangle$ – рассеянная:

$$|\psi\rangle = |\mathbf{k}\rangle + |\chi\rangle, \qquad \hat{H}_0|\mathbf{k}\rangle = E|\mathbf{k}\rangle$$

$$(\hat{H}_0+\hat{V})(|\mathbf{k}\rangle+|\chi\rangle) = E(|\mathbf{k}\rangle+|\chi\rangle) \to (E-\hat{H})|\chi\rangle = \hat{V}|\mathbf{k}\rangle$$
$$|\chi\rangle = (E-\hat{H})^{-1}\hat{V}|\mathbf{k}\rangle$$
$$\hat{G}_E: \qquad (E-\hat{H})\hat{G}_E \equiv \hat{\mathbb{I}}$$

$G_E(\mathbf{r},\mathbf{r}') := \langle \mathbf{r}|\hat{G}_E|\mathbf{r}'\rangle$,

$$(E-\hat{H})G_E(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')$$

$\hat{G}_E^{(0)} := (E-\hat{H}_0)^{-1}$,

$$G_E^{(0)}(\mathbf{r},\mathbf{r}') = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')}}{E-\frac{k^2}{2m}}, \qquad G_E^{(0,R)}(\mathbf{r},\mathbf{r}') = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')}}{E+i0-\frac{k^2}{2m}}$$

$$\hat{G}_E = (E-\hat{H})^{-1} = (E-\hat{H}_0-\hat{V})^{-1} = \hat{G}_E^{(0)} + \hat{G}_E^{(0)}\hat{V}\hat{G}_E^{(0)} + ...$$

$$|\chi\rangle = (E-\hat{H}+i0)^{-1}\hat{V}|\mathbf{k}\rangle =$$
$$= (\hat{G}_E^{(0,R)}\hat{V} + \hat{G}_E^{(0,R)}\hat{V}\hat{G}_E^{(0,R)}\hat{V} + ...)|\mathbf{k}\rangle =$$
$$= \hat{G}_E^{(0,R)}(\hat{V} + \hat{V}\hat{G}_E^{(0,R)}\hat{V} + ...)|\mathbf{k}\rangle = \hat{G}_E^{(0,R)}\hat{T}_E|\mathbf{k}\rangle$$

$$\hat{T}_E := \hat{V} + \hat{V}\hat{G}_E^{(0,R)}\hat{V} + ... = \hat{V}(1 - \hat{G}_E^{(0,R)}V)^{-1}$$

Finally,

$$\chi_{\mathbf{k}}(\mathbf{r}) = \langle \mathbf{r}|\chi\rangle = \langle \mathbf{r}|\hat{G}_E^{(0,R)}\hat{T}_E|\mathbf{k}\rangle = \int d\mathbf{r}'\frac{d\mathbf{k}'}{(2\pi)^d}\langle \mathbf{r}|\hat{G}_E^{(0,R)}|\mathbf{r}'\rangle\langle \mathbf{r}'|\mathbf{k}'\rangle\langle \mathbf{k}'|\hat{T}_E|\mathbf{k}\rangle =$$
$$= \int d\mathbf{r}'\frac{d\mathbf{k}'}{(2\pi)^d}\hat{G}_E^{(0,R)}(\mathbf{r},\mathbf{r}')e^{i\mathbf{k}'\mathbf{r}'}\hat{T}_E(\mathbf{k},\mathbf{k}')$$

$\hat{T}_{E\text{Brn}} \approx \hat{V}_{\text{Brn}}$,

$$\chi_{\mathbf{k}\text{Brn}}(\mathbf{r}) = \int d\mathbf{r}'\frac{d\mathbf{k}'}{(2\pi)^d}\hat{G}_E^{(0,R)}(\mathbf{r},\mathbf{r}')e^{i\mathbf{k}'\mathbf{r}'}\langle \mathbf{k}'|\hat{V}|\mathbf{k}\rangle$$

Solution. для 1D

$$G_{E\ 1D}^{(0,R)}(x) = \int\frac{dk}{2\pi}\frac{e^{ikx}}{E + i0 - \frac{k^2}{2m}} = \frac{m}{\pi}\int dk\frac{e^{ikx}}{2mE - k^2 + i0} = \frac{m}{\pi}2\pi i\operatorname*{res}_{k=+\sqrt{2mE}}\left(\frac{e^{ikx}}{2mE - k^2}\right) = -i\sqrt{\frac{m}{2E}}e^{i\sqrt{2mE}x}$$

Тут мы сместили контур чуть ниже оси и замкнули сверху. Только один вычет находился сверху над осью, второй после взятия корня попал под ось, ибо он равен $k_- = \sqrt{-2mE - i0}$, он не дает вклад в интеграл (?? да???).

$$G_E^{(0,R)}(x,x') = -\frac{im}{k_E}e^{ik_E|x-x'|}, \quad k_E = \sqrt{2mE} = k$$
$$\chi_k(x) = \int dx'\frac{dk'}{2\pi}\hat{G}_E^{(0,R)}(x,x')e^{ik'x'}\langle k'|\hat{V}|k\rangle = -\frac{im}{k}\int dx'\frac{dk'}{2\pi}e^{ik|x-x'|}e^{ik'x'}\tilde{V}_{k-k'}$$
$$|x - x'| \approx x - n_x x', \quad x \to \infty$$

$$\chi_k(x) = -\frac{im}{k}\int dx'\frac{dk'}{2\pi}e^{ik(x-n_x x')}e^{ik'x'}\tilde{V}_{k-k'} = -\frac{im}{k}\int dx'\delta(x')e^{ik(x-n_x x')}\tilde{V}_{k-k'} = -\frac{im}{k}e^{ikx}\tilde{V}_{k-k'}$$

$$f(n,n') = -\frac{m}{k}\tilde{V}_{k-k'} = \begin{cases} r = -\frac{m}{k}\int V(x)dx, & \mathbf{n}\uparrow\uparrow\mathbf{n}' \\ t = -\frac{m}{k}\int V(x)e^{2kx}dx, & \mathbf{n}\uparrow\downarrow\mathbf{n}' \end{cases}$$
$$\sigma = r^2 + t^2$$

Solution. для 2D (??)

$$G_{E\ 2D}^{(0,R)}(\mathbf{r}) = \int\frac{d^2\mathbf{k}}{(2\pi)^2}\frac{e^{i\mathbf{k}\mathbf{r}}}{E + i0 - \frac{k^2}{2m}} = \int\limits_0^\infty\frac{dkk}{4\pi^2}\frac{1}{E + i0 - \frac{k^2}{2m}}\int\limits_0^{2\pi}d\varphi e^{ikr\cos\varphi}$$

Воспользуемся методом стационарной фазы:

$$\int\limits_0^{2\pi}d\varphi e^{ikr\cos\varphi} \overset{kr\gg 1}{\approx} \sqrt{\frac{2\pi}{kr}}\left(e^{ikr - i\frac{\pi}{4}} + e^{-ikr + i\frac{\pi}{4}}\right) = 2\sqrt{\frac{2\pi}{kr}}\cos\left(kr - \frac{\pi}{4}\right),$$

$$G_{E\ 2D}^{(0,R)}(\mathbf{r}) = \frac{\sqrt{2\pi}}{2\pi^2\sqrt{r}}\int\limits_0^\infty\frac{dk\sqrt{k}\cos\left(kr - \frac{\pi}{4}\right)}{E + i0 - \frac{k^2}{2m}}$$

(!!!! из того, что тут написано не понять никогда переход. заново нужно решить и почитать годное место про это!!!!)

$$G_{E\ 2D}^{(0,R)}(\mathbf{r}) = \frac{m}{\sqrt{2\pi k_E r}}e^{ik_E r + i\frac{\pi}{4}} \qquad \Rightarrow \qquad G_{E\ 2D}^{(0,R)}(\mathbf{r},\mathbf{r}') = \frac{m}{\sqrt{2\pi k_E r}}e^{ik_E|\mathbf{r}-\mathbf{r}'| + i\frac{\pi}{4}}$$

(??? почему косинус стал экспонентой?? не понимаю, почему по большому контуру интеграл ноль, там же экспоненты появляются?)

$$\chi_{\mathbf{k}}(\mathbf{r}) = \int d\mathbf{r}' \frac{d\mathbf{k}'}{(2\pi)^2} G_{E\ 2D}^{(0,R)}(\mathbf{r},\mathbf{r}')\ e^{i\mathbf{k}'\mathbf{r}'}\ \langle \mathbf{k}'|\hat{V}|\mathbf{k}\rangle = \frac{m}{\sqrt{2\pi kr}} \int d\mathbf{r}' \delta(\mathbf{r}') e^{ik|\mathbf{r}-\mathbf{r}'|+i\frac{\pi}{4}} e^{i\mathbf{k}'\mathbf{r}'} \tilde{V}_{\mathbf{k}-\mathbf{k}'} = \frac{m}{\sqrt{2\pi kr}} e^{ikr+i\frac{\pi}{4}} \tilde{V}_{\mathbf{k}-\mathbf{k}'}$$

$$f(\mathbf{n},\mathbf{n}') = \frac{m}{\sqrt{2\pi k}} \tilde{V}_{\mathbf{k}-\mathbf{k}'}$$

$$d\sigma = |f(\mathbf{n},\mathbf{n}')|^2 d\theta$$

ПТФ-13.з2. Рассеяние на $\frac{1}{a+|x|}$

Рассмотрите рассеяние медленных частиц на одномерном потенциале $V(x) = -V_0 \frac{a}{a+|x|}$. Используя

$$f(n,n') = -\frac{m}{k}\tilde{V}_{k-k'} = \begin{cases} r = -\frac{m}{k}\int V(x)dx, & \mathbf{n} \uparrow\uparrow \mathbf{n}', \\ t = -\frac{m}{k}\int V(x)e^{2kx}dx, & \mathbf{n} \uparrow\downarrow \mathbf{n}', \end{cases}$$

вычислите коэффициент прохождения частиц в ведущем Борновском приближении.

Solution.

Если воспользоваться формулой из предыдущей задачи, то

$$t = -\frac{m}{k}\int V(x)dx = -\frac{m}{k}V_0 \int \frac{adx}{a+|x|}$$

Интеграл расходится. Воспользуемся предыдущей формулой, при этом обрезав интеграл по $[-R;R]$, для какого-то $R > 0$.

$$\chi_k(x) = -i\frac{m}{k}\int\limits_{-R}^{R} e^{ik|x-x'|}V(x')e^{ikx'}dx', \quad x > R$$

$$\chi_k(x) \quad = \quad 2iV_0 a e^{ikx}\frac{m}{k}\int\limits_0^R \frac{dx'}{x'+a} \quad = \quad 2iV_0 a e^{ikx}\frac{m}{k}\ln\frac{a+R}{a} \quad = \quad 2iV_0 a e^{ikx}\frac{m}{k}(\ln(ka\ +\ kR)\ -\ \ln ka)$$

k был вставлен в логарифм дополнительно.

Частицы медленные, $ka \ll 1$,

$$R \sim \frac{1}{k} \gg a, \quad \ln(ka+kR) \approx \ln ka$$

(???? почему так????) Мб тут мы говорим, что первый логарифм гораздо больше второго, но тем не менее, почему он зависит только от a по итогу????

$$\chi_k(x) = -2iV_0 a e^{ikx}\frac{m}{k}\ln ka$$

$$t = -2V_0 a\sqrt{\frac{m}{2E}}\ln ka = -\frac{V_0}{E}ka\ln ka$$

Сечение рассеяния в кулоновском поле

Найти в борновском приближении дифференциальное сечение рассеяния частиц кулоновским полем с произвольным зарядом. Указать условия его применимости.

Solution.

Это типичная задача теории (пусть и нетривиальная), можно написать ответ сразу, но ниже короткое решение еще есть.

$$f(\theta) = -\frac{2\mu}{\hbar^2 q}\int\limits_0^\infty r' V\left(r'\right)\sin\left(qr'\right)dr'$$

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{4\mu^2}{\hbar^4 q^2}\left|\int\limits_0^\infty r' V\left(r'\right)\sin\left(qr'\right)dr'\right|^2$$

$$V(r) = Z_1 Z_2 e^2/r$$

$$\int\limits_0^\infty \sin(qr)dr = \lim_{\lambda\to 0}\int\limits_0^\infty e^{-\lambda r}\sin(qr)dr = \frac{1}{2i}\lim_{\lambda\to 0}\left[\int\limits_0^\infty e^{-(\lambda-iq)r}dr - \int\limits_0^\infty e^{-(\lambda+iq)r}dr\right]$$
$$= \frac{1}{2i}\lim_{\lambda\to 0}\left[\frac{1}{\lambda-iq} - \frac{1}{\lambda+iq}\right] = \frac{1}{q}$$

$q = 2k\sin(\theta/2)$,

$$\frac{d\sigma}{d\Omega} = \left(\frac{2Z_1\mu Z_2 e^2}{\hbar^2 q^2}\right)^2 = \left(\frac{Z_1 Z_2 \mu e^2}{2\hbar^2 k^2}\right)^2 \sin^{-4}\left(\frac{\theta}{2}\right) = \frac{Z_1^2 Z_2^2 e^4}{16E^2}\sin^{-4}\left(\frac{\theta}{2}\right),$$

$E := \hbar^2 k^2/2\mu$ (Rutherford's formula).

Условия применимости борновсокго приближения для Кулона

The first Born approximation is valid whenever the wave function $\Psi(r)$ is only slightly different from the incident plane wave; that is, whenever the second term in (1.23) is very small compared to the first:

$$\psi(\vec{r}) \simeq \phi_{inc}(\vec{r}) - \frac{\mu}{2\pi\hbar^2}\int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}V\left(\vec{r}'\right)\phi_{inc}\left(\vec{r}'\right)d^3r'.$$
$$|\frac{\mu}{2\pi\hbar^2}\int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}V\left(r'\right)e^{i\vec{k}_0\cdot\vec{r}'}d^3r'| \ll |\phi_{inc}(\vec{r})|.$$

Since $\phi_{inc} = e^{i\vec{k}_0\cdot\vec{r}}$ we have

$$|\frac{\mu}{2\pi\hbar^2}\int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}V\left(r'\right)e^{i\vec{k}_0\cdot\vec{r}'}d^3r'| \ll 1.$$

In elastic scattering $k_0 = k$ and assuming that the scattering potential is largest near $r = 0$, we have

$$|\frac{\mu}{\hbar^2}\int\limits_0^\infty r' e^{ik\vec{r}'}V\left(r'\right)dr'\int\limits_0^\pi e^{ikr'\cos\theta'}\sin\theta' d\theta'| \ll 1$$
$$\frac{\mu}{\hbar^2 k}|\int\limits_0^\infty V\left(r'\right)\left(e^{2ikr'}-1\right)dr'| \ll 1.$$

17.4 Specific qeuestions and setups for scattering

17.4.1 Problems about low-energy scattering and resonant scattering 1

GKKG.13.27 Potential $1/r^\nu, 2 < \nu \leq 3$

Find the energy dependence of the scattering cross-section, $\sigma(E)$, in a field that decreases at large distances as $U(r) \approx \alpha/r^\nu, 2 < \nu \leq 3$, and in the low-energy limit, $E \to 0$.

Solution

For potentials with this behavior at large distances, the Born amplitude for $q \to 0$ diverges. Since $q = 2k\sin(\theta/2)$, then for $E \to 0$ in the Born approximation, the total scattering cross-section would diverge as well (here, $q \to 0$ for all scattering angles). The divergence of the scattering cross-section signals the importance of large distances, where conditions (XIII.7) are fulfilled, and therefore the Born approximation does work. Here, according to Eq. (XIII.12), we have:

$$f(q) \approx -\frac{2m\alpha}{\hbar^2 q^{3-\nu}} \int\limits_{qR}^{\infty} \frac{\sin x}{x^{\nu-1}} dx \tag{1}$$

We consider only the diverging part of the amplitude and total scattering cross-section. We do not consider a contribution from distances $r \leq R$, where the potential is not described by its known asymptote.

For $\nu < 3$, in Eq. (1) we set the lower integration limit as $qR = 0$ and obtain:

$$f = \frac{C_\nu}{q^{3-\nu}}, \quad C_\nu = \frac{\pi m\alpha}{\hbar^2 \Gamma(\nu-1)\cos(\pi\nu/2)} \tag{2}$$

using the integral

$$\int\limits_0^{\infty} \frac{\sin x}{x^{\nu-1}} dx = \Gamma(2-\nu)\sin\frac{\pi\nu}{2} = -\frac{\pi\sin(\pi\nu/2)}{\Gamma(\nu-1)\sin\pi\nu}$$

The total scattering cross-section is (for $q^2 = 2k^2(1-\cos\theta)$)

$$\sigma = 2\pi \int\limits_0^{\pi} f^2 \sin\theta d\theta \underset{E\to 0}{\approx} 2\pi C_\nu^2 \left(\frac{\hbar^2}{4mE}\right)^{3-\nu} \int\limits_{-1}^{1} \frac{dz}{(1-z)^{3-\nu}} \propto \frac{1}{E^{3-\nu}} \to \infty \tag{3}$$

If $\nu = 3$, we cannot replace the lower limit of integration in Eq. (1) by zero, due to integral divergence. Since $\sin x \approx x$ for $x \to 0$, the diverging part of the integral is equal to $\ln(1/qR)$, so that

$$f \approx \frac{2m\alpha}{\hbar^2} \ln qR \tag{4}$$

and the total scattering cross-section is

$$\sigma = \int f^2 d\Omega \approx \int \frac{4m^2\alpha^2}{\hbar^4} \ln^2 kR d\Omega = \frac{16\pi m^2\alpha^2}{\hbar^4} \ln^2 kR \to \infty \tag{5}$$

For a calculation of the diverging, $\propto \ln^2 k$, part of the scattering cross-section, we put $\ln qR \approx \ln kR$. An uncertainty in the value of R gives rise to the logarithmic accuracy of Eqs. (4) and (5).

GKKG.13.28

Find the k-dependence of the phase shifts, $\delta_l(k)$, for slow particles, and discuss the effective-range expansion in the Born approximation. What are the constraints on the large-distance asymptotic behavior of the potential that ensure the applicability of the expansion (XIII.15)? Introduce the following parameters of low-energy scattering: scattering length, a_l, and an effective range of the interaction, r_l, with the angular momentum, l.

Solution

For $k \to 0$, the argument, $x = kr$, of the Bessel function in Eq. (XIII.12) is small, and we can use the known expansion of $J_\mu(x)$ for $x \to 0$. We consider only the first two terms of the expansion, [333] and obtain

$$\delta_l^B(k) \approx k^{2l+1}\left[A_l + B_l k^2 + ...\right] \propto k^{2l+1} \tag{1}$$

Here,

$$A_l = c_l \int\limits_0^{\infty} U(r) r^{2l+2} dr, \quad B_l = -\frac{c_l}{2l+3} \int\limits_0^{\infty} U(r) r^{2l+4} dr$$

$$c_l = -\frac{\pi m}{2^{2l+1}\Gamma^2(l+3/2)\hbar^2} \tag{2}$$

Taking into account the effective range expansion, Eq. (XIII.15), and also the smallness of the phase shift in the Born approximation, we find:

$$a_l^B = -A_l, \quad r_l^B = -2B_l A_l^{-2} \tag{3}$$

One of the applicability conditions for these results is a fast decrease of the potential at large distances. This guarantees convergence of the integral in Eq. (2). For an exponential decrease of the potential, no restriction on the values [334] of l appears.

For potentials with a power-law decrease, $U \approx \alpha/r^\nu$, we have a different situation. For the values $l < (\nu-5)/2$, the integrals in Eq. (2) converge in the upper limit, and the notions of the scattering length a_l and effective range r_l are still well-defined.

In the case of $(\nu-5)/2 \le l < (\nu-3)/2$, the second of the integrals in Eq. (2) diverges. Here, the effective range expansion, Eq. (XIII.15), is not valid, but the notion of the scattering length and the dependence $\delta_l \approx -a_l k^{2l+1}$ for slow particles are preserved.

Finally, for the values $l \ge (\nu-3)/2$, the dependence $\delta_l \propto k^{2l+1}$ is broken for $k \to 0$. Low-energy scattering with an arbitrary angular momentum l in potentials with a power "tail" is considered in the following two problems (see Problem 13.27).

GKKG.13.29

For a potential with a power-law decrease at large distances, $U \approx \alpha/r^\nu$ with $\nu > 2$, find the k-dependence of phase-shifts for slow particles with an angular momentum, l.

Solution

For the values $l < (\nu-3)/2, \delta_l = A_l k^{2l+1}$. In the Born approximation, the coefficient A_l in this case is obtained as in the previous problem. In the case $l \ge (\nu-3)/2$, we can not replace the Bessel function, $J_\mu(x)$, in Eq. (XIII.12) by its first, $\propto x^\mu$, expansion term, as it would have led the dependence $\delta_l \propto k^{2l+1}$, and a divergence in the integral. Now, we divide the integration domain in Eq. (XIII.12) into two parts: from $r = 0$ to $r = R$, and from $r = R$ to $r = \infty$ (the value of R is such that for $r > R$, we can use an asymptotic form of the potential), we see that the first integral, proportional to k^{2l+1}, is less important than the second one. We find:

$$\delta_l \approx -\frac{\pi m\alpha}{\hbar^2} k^{\nu-2} \int\limits_{kR}^{\infty} \frac{1}{x^{\nu-1}} J_{l+1/2}^2(x)dx \tag{1}$$

For $l > (\nu-3)/2$, we can replace the lower integration limit by zero and obtain:

$$\delta_l \approx -\frac{\pi m\alpha}{\hbar^2} \frac{\Gamma(\nu-1)\Gamma(l+(3-\nu)/2)}{2^{\nu-1}\Gamma^2(\nu/2)\Gamma(l+(\nu+1)/2)} k^{\nu-2} \tag{2}$$

In the case of $l = (\nu-3)/2$, the integral in Eq. (1) for $k \to 0$ diverges in the lower limit. Using the expansion of $J_\mu(x)$ for $x \to 0$, we find the divergent part of the integral and the phase shift:

$$\delta_l \approx \frac{\pi m\alpha}{2^{2l+1}\Gamma^2(l+3/2)} k^{2l+1} \ln kR \tag{3}$$

Let us make a few remarks:

1. Although the above results are based on the Born approximation, for $\nu > 2$ they apply more broadly. Indeed, in this case, the large distances are essential, where $|U(r)| \ll \hbar^2/mr^2$, so that the potential can be considered as a perturbation.

2. For a potential that is a superposition of a "strong" short-range and a "weak" long-range (with a power-law asymptote) potential, generally speaking, [335] the contributions to the phase shift are additive: $\delta_l \approx \delta_{l,\,\mathrm{shor}} + \delta_{l,long}$. For abnormally small k, the dominant contribution comes from the long-range potential, while for k not too small it comes from the short-range potential. See Problem 13.37, and also Problem 13.42.

[0] [333] These transformations are valid for fixed finite value of k, but $l \gg (kR)^2$, which allows us to make a conclusion for the phase shifts at large values of the angular momentum: $\delta_l \propto (kR/l)^{2l+1}$.

[334] The dependence $\delta_l \propto k^{2l+1}$ is valid for "strong" potentials including those for which the Born approximation is not valid.

GKKG.13.30

For potential with a power-law decrease at large distances, $U \approx \alpha/r^\nu$, discuss how the effective-range expansion, see Eq. (XIII.15), should be modified in order to describe scattering of particles with angular momenta, l, in the range $(\nu-5)/2 \le l < (\nu$ - $3)/2$. As an illustration of this result, consider s-wave scattering of slow particles in a potential with the large-distance asymptote, $U \approx \alpha/r^4$.

Solution

Taking into account the solutions of the two previous problems, it is easy to obtain the following expansions:

$$\delta_l + a_l k^{2l+1} \approx -\frac{\pi m\alpha}{\hbar^2} k^{\nu-2} \int\limits_0^\infty \frac{1}{x^{\nu-1}} \left[J^2_{l+1/2}(x) - \frac{x^{2l+1}}{2^{2l+1}\Gamma^2(l+3/2)} \right] dx$$

$$\frac{\nu-5}{2} < l < \frac{\nu-3}{2} \tag{1}$$

In the case $l = (\nu-5)/2$, we can also obtain Eq. (1), but the lower limit of the integral will be equal to kR. Calculating the divergent part, we find:

$$\delta_l + a_l k^{2l+1} \approx -\frac{\pi m\alpha}{2^{2l+1}(2l+3)\Gamma^2(l+3/2)} k^{2l+3} \ln kR \tag{2}$$

In particular, for a potential that at large distances has the form $U \approx \alpha/r^4$(i.e., $\nu = 4$), and for $l = 0$, we obtain from Eq. (1):

$$\delta_0 + a_0 k \approx -\frac{2m\alpha}{\hbar^2} k^2 \int\limits_0^\infty \frac{1}{x^3} \left[\frac{\sin^2 x}{x} - x \right] dx = \frac{2\pi m\alpha}{3\hbar^2} k^2$$

The generalization of the effective range expansion, Eq. (XIII.15), takes the form:

$$k \cot \delta_0(k) \approx -\frac{1}{a_0} + \frac{2\pi m\alpha}{3\hbar^2 a_0^2} k$$

GKKG.13.31 Catalog of scattering lengths

Find the scattering length, a_0, in the following potentials:

a) $U(r) = \begin{cases} -U_0, & r < R, \\ 0, & r > R \end{cases}$ b) $U(r) = -U_0 R\delta(r-R)$; c) $U(r) = -U_0 e^{-r/R}$

d) $U(r) = -U_0 \left[1 + (r/R)^2\right]^{-2}$; e) $U(r) = U_0(R/r)^4$, $U_0 > 0$.

What is notable about the potential parameters that correspond to a divergent scattering length?

What is the reason behind a non-analytic dependence of $a_0\,(U_0)$ on the parameter U_0, for $U_0 \to 0$ in case e)?

Solution

To calculate the scattering length, a_0, we should find a bounded solution of the radial Schrdinger equation with $E = 0$ and $l = 0$. Its asymptote, [336]

$$R_{l=0,E=0} \approx 1 - \frac{a_0}{r} \quad \text{for} \quad r \to \infty$$

determines the value of a_0. The solutions of the Schrdinger equation for the potentials considered were discussed in Chapter 4, so here we make only several remarks, [337] (below, $\chi = rR_{l=0,E=0}$ and $\lambda = \sqrt{2mU_0R^2/\hbar^2}$).

a) For the square potential well,

$$\chi = \begin{cases} A \sin \frac{\lambda r}{R}, & r < R \\ r - a_0, & r > R \end{cases}$$

From the conditions of χ and χ' continuity at the point $r = R$, we find:

$$a_0 = \left(1 - \frac{1}{\lambda} \tan \lambda\right) R$$

[336] Such an asymptote assumes a decrease of the potential at large distances faster than $\propto 1/r^3$.

[337] Let us reiterate that the boundary condition, $\psi(\infty) = 0$, that is used for states of the discrete spectrum, does not appear here.
b) For the δ-spherical potential,

$$\chi = \begin{cases} Cr, & r < R \\ a_0 - r, r > R \end{cases}$$

Matching the solution at the point $r = R$ (see Problem 4.8) gives

$$a_0 = -\frac{\lambda^2}{1-\lambda^2} R$$

c) For an exponential potential, the solution to the Schrdinger equation is

$$\chi = J_0(2\lambda)N_0(x) - N_0(2\lambda)J_0(x), \text{ where } x = 2\lambda e^{-r/2R}$$

Here, J_0 and N_0 are Bessel and Neumann functions, respectively. We have used the boundary condition $\chi(r = 0) = 0$ (compare to Problem 4.8). Since for $r \to \infty$, we have $x \to 0$, then we can use the expression (with $\mathcal{C} = e^\gamma = 1.781..., \gamma = 0.5772...$ is Euler's constant):

$$J_0(x) \approx 1 - \frac{x^2}{4}, \quad N_0(x) \approx \frac{2}{\pi} J_0(x) \ln \frac{x}{2} + \frac{2\gamma}{\pi} + \frac{1}{2\pi}(1-\gamma)x^2, \quad |x| \ll 1$$

and find the scattering length:

$$a_0 = \frac{\pi R}{J_0(2\lambda)} \left[\frac{2}{\pi} J_0(2\lambda) \ln \gamma\lambda - N_0(2\lambda) \right] \tag{3}$$

d) For the potential given, the Schrdinger equation has the form (compare with Problem 4.25):

$$\psi_{E=0,l=0} = C\sqrt{1 + \frac{R^2}{r^2}} \sin\left(\xi \arctan \frac{r}{R}\right)$$

where $\xi = \sqrt{1+\lambda^2}$. From its asymptote, we find:

$$a_0 = \xi R \cot\left(\frac{1}{2}\pi\xi\right) \tag{4}$$

e) In analogy to the solution to Problem 4.25, we find the wavefunction,

$$\psi_{E=0,l=0} = A \exp\left\{-\frac{\lambda R}{r}\right\}$$

and the scattering length,

$$a_0 = \lambda R \tag{5}$$

Now, we discuss the results obtained. We first mention an essential difference in the dependence of the scattering length, a_0, on the parameter $\lambda \propto \sqrt{U_0}$ for $U_0 \to 0$ in case e) in comparison to the other cases a) -d). According to (1)-(4), a_0 for small λ is expanded into a series in powers of λ^2, and is an analytic function of the parameter
U_0. Depending on the sign of U_0, these expressions give a scattering length in either an attractive potential $U_0 > 0$, or a repulsive one $U_0 < 0$. For example, Eq. (1) for $U_0 < 0$ takes the form:

$$a_0 = \left(1 - \frac{1}{|\lambda|} \tanh|\lambda|\right) R$$

and describes the scattering length of a potential barrier. In the case of the potential $U = \alpha/r^4$, with $\alpha = U_0 R^4$, the dependence of a_0 on the parameter α (or, equivalently, U_0) is non-analytic, since $a_0 \propto \sqrt{\alpha}$. This non-analyticity reflects a qualitatively different way in which the potential affects the particle for small values of $\alpha > 0$ versus $\alpha < 0$, that manifests itself in the "fall into the center" phenomenon in the latter case [338]$\alpha < 0$. Here, Eq. (5) is invalid, since the boundary condition, $\psi(0) = 0$, used for its derivation, could not be fulfilled and requires a modification. Compare to Problem 9.14.

Eqs. (1)-(4) reflect the general nature of the dependence of the scattering length, a_0, on the parameters U_0 and R for a regular potential of a fixed sign and of the form $U(r) = -U_0 f(r/R)$, where $f(|z|) \geq 0$ (attraction

for $U_0 > 0$ and repulsion for $U_0 < 0$). Its qualitative nature is shown in Fig. 13.3.

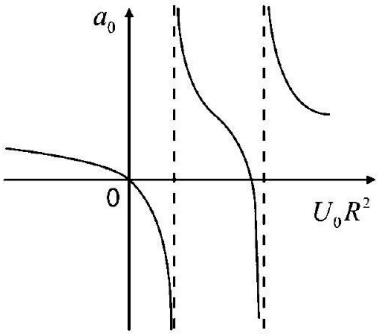


Fig. 13.3

We now list some properties of the solution:

1. For $|\lambda|^2 \ll 1$ (a "weak" potential), the scattering length is also small, since $|a_0| \sim |\lambda|^2 R \ll R$. Writing $a_0 = -\beta\lambda^2 R$ from a) -d), we find that the parameter β, is equal to $1/3, 1, 2, \pi/4$ respectively. These results can be obtained from the Born approximation equation:

$$a_0^B = -f^B(E=0) = \frac{m}{2\pi\hbar^2}\int U(r)dV$$

The sign of the scattering length coincides with the sign of potential.

2) For an increase of $|\lambda|^2$, the value of the scattering length increases. The dependence of a_0 on U_0 is monotonic, except for the unique values, λ_n, of the parameter λ, where, in an attractive potential, the scattering length, a_0, becomes infinite. Such values of λ correspond to the appearance of a new bound state in the potential with the angular momentum $l = 0$.[339] Indeed, the wavefunction's asymptote for $r \to \infty$ at the threshold of emergence of a new bound state is $\psi_{E=0} \propto 1/r$ (but not $C_1 + C_2/r$, as in the general case; compare to Problem 4.25). This corresponds to a divergent scattering length, $a_0 \to \infty$.

Let us prove that the dependence of a_0 on U_0 is monotonous if the potential does not change sign. The two Schrdinger equations for $E = 0$ and $l = 0$ are

$$\chi_0'' = -\frac{2m}{\hbar^2}U_0 f\left(\frac{r}{R}\right)\chi_0, \quad \chi'' = -\frac{2m}{\hbar^2}\left(U_0 + \delta U_0\right) f\left(\frac{r}{R}\right)\chi$$

The boundary conditions take the form $\chi_0(0) = \chi(0) = 0$, while the asymptotes of the solutions for $r \to \infty$ are $\chi_0 \approx a_0 - r$ and $\chi \approx a - r$, with $a = a_0 + \delta a_0$ (where δa_0 is a change in the s-wave scattering length due to a change of the potential by $-\delta U_0 f$). Multiplying the first of these equations by χ and the second one by χ_0, subtracting them term by term, and integrating over r from 0 to ∞, we find:

$$\delta a_0 = -\left(\chi\chi_0' - \chi_0\chi'\right)\Big|_0^\infty \approx -\frac{2m}{\hbar^2}\delta U_0 \int\limits_0^\infty f\left(\frac{r}{R}\right)\chi_0^2(r)dr$$

In the integral, we put $\chi \approx \chi_0$, which is valid due to the assumed smallness of $\delta U_0 \to 0$ and the condition $a_0 \neq \infty$; here, δa_0 is also small and $\delta a_0/\delta U_0 < 0$, which proves the monotonic $a_0\,(U_0)$ dependence.

3) Along with the values of λ close to λ_n, for which the scattering amplitude is anomalously large (resonant scattering), there also exist values $\tilde{\lambda}_n$, where the scattering length on the contrary vanishes. For such values, $\tilde{\lambda}_n$, of the parameters of the potential, the scattering cross-section, $\sigma = 4\pi a_0^2$, of particles with energy $E = 0$ vanishes. So for λ close to $\tilde{\lambda}_n$, the scattering cross-section for slow particles, $kR \ll 1$, can be abnormally small, which manifests itself in the Ramsauer-Townsend effect. Let us emphasize that this smallness of the scattering cross-section, $\sigma \ll \pi R^2$, for slow particles in a "strong" short-range potential of radius R might appear only if the potential is attractive.

Finally, let us mention the following property of the scattering length in the case of a strong potential, with $|\lambda| \gg 1$. If the potential has a well-defined radius, R, as in the case of a rectangular δ-well (or the corresponding barrier), then $a_0 \approx R$, except for narrow regions of λ in the vicinity of the points [340]λ_n (see Eqs. (1) and (2)). This property exists also for rapidly (exponentially) decreasing

[339] In the case of the δ-well, Eq. (2), only one bound state with the angular momentum $l = 0$ appears, as $\lambda \geq \lambda_0 = 1$.

[340] These narrow regions also include the points $\tilde{\lambda}_n$. As is seen from Eqs. (1) and (3), for rapidly decreasing potentials, the points λ_n and $\tilde{\lambda}_n$ move closer as $n \to \infty$; for the step potential (see Eq. (4)) this

[0][338] Compare to the analogous property of the scattering phases δ_l, in the case of an attractive potential $U = -|\alpha|/r^2$, which follows from Eq. (1) of Problem 13.19. For $2m|\alpha|/\hbar^2 = (l + 1/2)^2$, the particle with the angular momentum, l, "falls into the center."

statement is not valid.
potentials. From Eq. (3), for $\ln \gamma\lambda \gg 1$, we have $a_0 \approx R_{eff} \approx 2R \ln \gamma\lambda$, except when the Bessel function, $J_0(2\lambda)$, is close to zero. These exceptional values of λ correspond to the appearance of new bound states. The difference from the previous case lies in the weak, logarithmic dependence of R_{eff} on λ, which is seen from the expression $|U(R_{eff})| \approx \hbar^2/mR_{\text{eff}}^2$. For potentials with a power-law decrease, as seen from Eq. (4), we have a different situation. In this case, $a_0(\lambda)$ is a "lively" function of λ in the entire interval between λ_n and λ_{n+1}.

GKKG.13.32 Scattering by ellipsoid

Find the scattering length and cross-section for slow particles scattered by an impenetrable ellipsoid, i.e., by the potential:

$$U(r) = \begin{cases} \infty, \frac{x^2+y^2}{b^2} + \frac{z^2}{c^2} < 1 \\ 0, \frac{x^2+y^2}{b^2} + \frac{z^2}{c^2} \geq 1 \end{cases}$$

Assume $c \geq b$. Consider specifically two limiting cases: $c \approx b$ and $c \gg b$.

Solution

This problem is reduced to solving the Schrdinger equation with energy $E = 0$, which takes the form $\Delta\psi(\mathbf{r}) = 0$ with the boundary condition $\psi(\mathbf{r}_0) = 0$ on the surface of the ellipsoid and with the asymptote, $\psi \approx 1 - a_0/r$, at large distances. The scattering length is [341] $a_0 = -f(E = 0)$.

For the function $\phi(\mathbf{r}) = 1 - \psi(\mathbf{r})$, the equation, the boundary condition, and the asymptote are:

$$\Delta\varphi = 0, \quad \varphi(\mathbf{r}_0) = 1, \quad \varphi \approx \frac{a_0}{r} \text{ for } r \to \infty \tag{1}$$

According to these relations, the function $\varphi(\mathbf{r})$ can be considered as an electrostatic potential of a charged ellipsoid that on its surface takes the value $\varphi_0 = 1$, and $e = a_0$ is the ellipsoid's total charge. Since $e = C\varphi_0$, where C is the capacitance, the particle's scattering length for an "impenetrable" ellipsoid is formally equivalent to the electrostatic capacitance of a conductor of the same form. [342] The solution of the electrostatic problem, Eq. (1), for an oblong ellipsoid is known and has the form (for $c > b$):

$$\varphi(\mathbf{r}) = \frac{e}{2\sqrt{c^2-b^2}} \ln \frac{z + \sqrt{c^2-b^2} + \left[\left(z + \sqrt{c^2-b^2}\right)^2 + x^2 + y^2\right]^{1/2}}{z - \sqrt{c^2-b^2} + \left[\left(z - \sqrt{c^2-b^2}\right)^2 + x^2 + y^2\right]^{1/2}} \tag{2}$$

[341] Let us emphasize that in the limit of zero energy, particle scattering is isotropic even in the case of a non-spherically-symmetric short-range interaction.

[342] The relation $a_0 = C$ is valid for an "impenetrable" body of an arbitrary form. For example, for particle scattering from an impenetrable disc of radius R, the scattering cross-section is $\sigma(E = 0) = (16/\pi)R^2$ (the disc capacitance is $C = 2R/\pi$).

This result can be obtained by the method of images: the potential created by the ellipsoid coincides with that of a homogeneously-charged segment, whose ends are at the foci of the ellipsoid, with the coordinates $x = y = 0, z = \pm\sqrt{c^2-b^2}$. Determining e from the condition $\varphi(\mathbf{r}_0) = 1$ (here, it is convenient to chose the point on the ellipsoid that lies on the rotation axis, $x = y = 0, z = c$), we find the scattering length:

$$a_0 = e = 2\sqrt{c^2-b^2} \left[\ln \frac{c + \sqrt{c^2-b^2}}{c - \sqrt{c^2-b^2}}\right]^{-1} \tag{3}$$

In the case $c = b$, we have $a_0 = c$ and $\sigma = 4\pi c^2$, the known result for slow particle scattering cross-section for an impenetrable sphere of radius $R = c$. For a strongly prolate ellipsoid, $c \gg b$, Eq. (3) gives:

$$a_0 \approx \frac{c}{\ln(2c/b)}, \quad \sigma(E = 0) \approx \frac{4\pi c^2}{(\ln(2c/b))^2} \tag{4}$$

The generalization to the case of an oblate ellipsoid, $b > c$, can be obtained using analytic continuation of the scattering length (3). Writing $\sqrt{c^2-b^2} = i\sqrt{b^2-c^2} \equiv iv$ and using the relation

$$\ln(c \pm iv) = \frac{1}{2}\ln\left(c^2 + v^2\right) \pm i \arctan\frac{v}{c}$$

we obtain

$$\ln\left(\frac{c+iv}{c-iv}\right) = 2i \arctan\frac{v}{c} = 2i \arctan\frac{\sqrt{b^2-c^2}}{c} = 2i \arccos\frac{c}{b}$$

and for the scattering length, we obtain ($b > c$)

$$a_0 = \frac{\sqrt{b^2 - c^2}}{\arccos(c/b)} \tag{5}$$

If we put here $c = 0$ and $b = R$, we obtain the scattering length, $a_0 = 2R/\pi$, for an impenetrable disc of radius R.

GKKG.13.33

In the quasi-classical approximation, find the scattering length, a_0, for a repulsive potential that has the asymptotic behavior $U \approx \alpha/r^4$ at large distances.

To illustrate the quasi-classical result obtained, apply it to the potentials a) $U = \alpha\left(R^2 + r^2\right)^{-2}$ and, b) $U = \alpha(R + r)^{-4}$, where $R > 0$. Compare these with exact results.

Solution

At finite distances, the quasi-classical solution of Eq. (IV.5) for the function $\chi = rR(r)$ with $E = 0$ and $l = 0$ should be chosen as follows

$$\chi_{quas}(r) = \frac{C}{\sqrt{|p|}} \exp\left\{-\frac{1}{\hbar}\int_r^\infty |p|dr\right\}, \quad |p| = \sqrt{2mU(r)} \tag{1}$$

Here, only the wavefunction that vanishes at the origin is kept. By neglecting the increasing part of the solution, we enforce the boundary condition, [343] $\chi(0) = 0$.

But at large distances, $r \to \infty$, we have $|p(r)| \propto 1/r^2 \to 0$, and the quasiclassical approximation is not applicable. So, we should match solution (1) at large distances, where $U \approx \alpha/r^4$, with the exact solution of the Schrdinger equation, whose asymptote, $\chi(r) \approx a_0 - r$, gives the scattering length. Such an exact solution has the form (see Problem 4.25):

$$\chi = r\left[\frac{a_0}{d}\sinh\frac{d}{r} - \cosh\frac{d}{r}\right]_{r\to\infty} \underset{\sim}{\approx} a_0 - r, \quad d = \sqrt{\frac{2m\alpha}{\hbar^2}} \tag{2}$$

Matching of the solutions (1) and (2) can be performed only if in Eq. (2), as well as in Eq. (1), there exists no term exponentially increasing towards the origin, $r \to 0$. Hence, we find the scattering length in the quasi-classical approximation:

$$a_{0,\ \text{quas}} = d = \sqrt{\frac{2m\alpha}{\hbar^2}} \tag{3}$$

This result for $U = \alpha/r^4$ reproduces the exact one.

For the other potentials from the problem condition, the scattering lengths are (see Problem 13.31d; $\xi = \sqrt{2m\alpha/\hbar^2R^2} = d/R$):

$$\text{a)}\ a_0 = R\sqrt{\xi^2 - 1}\coth\left(\frac{1}{2}\pi\sqrt{\xi^2 - 1}\right),\ \text{b)}\ a_0 = R\xi\left(\coth\xi - \frac{1}{\xi}\right) \tag{4}$$

As expected, for $\xi \to \infty$ they become Eq. (3). Even for the values $\xi \geq 1$, the quasiclassical result is close to the exact one. As an illustration, below is a table showing the ratios, $\eta = a_{0,\ \text{quas}}/a_0$ for several ξ:

ξ	1	2	4	6
$\eta, a)$	1.571	1.145	1.033	1.014
$\eta, b)$	3.202	1.862	1.332	1.200

[343] If $U(r)$ is a bounded potential, $\chi_{quas}(0)$ is different from zero, but is exponentially small. Such a break-down of the boundary condition gives exponentially small errors in the results for relevant observables. More important are corrections connected to the deviation of the potential from its asymptotic form at large distances. See the following problem.

The lower accuracy in case b is due to a larger difference between the potential $U(r)$ and its asymptote, α/r^4, at large distances. See the following problem.

GKKG.13.34

In the conditions of the previous problem, find a quasi-classical correction to the scattering length using the subleading term in the large-distance expansion of the potential: $U = \alpha r^{-4}(1 + b/r + \ldots)$.

Solution

If the potential $U(r)$ differs from α/r^4 only at finite distances, $r \le R$, then for $\xi = \sqrt{2m\alpha/\hbar^2 R^2} \gg 1$, the difference of a_0 from its quasi-classical value $\sqrt{2m\alpha/\hbar^2}$ is exponentially small and is outside the limits of applicability of the quasi-classical approximation.

If the difference, $U(r) - \alpha/r^4$, is different from zero for $r > R$, then power-law corrections in the parameter, $1/\xi \propto \hbar$, appear. To determine the first such correction in the case of $U(r) \approx \left(\alpha/r^4\right)(1 + b/r)$ for $r \to \infty$, it is necessary to find a solution of the Schrdinger equation at large distances, whose accuracy allows to determine correctly a correction in the asymptote of the potential. To do this, we note that within the required accuracy, $U = \alpha/(r - b/4)^4$. For this potential, the Schrdinger equation allows an exact solution, which can be obtained by replacing r by $r - b/4$ in Eq. (2) of the previous problem, and has the form:

$$\chi = -\left(r - \frac{b}{4}\right) \exp\left\{-\frac{\sqrt{2m\alpha}}{\hbar(r - b/4)}\right\} \tag{1}$$

We have omitted here a second independent solution of the Schrdinger equation, which increases exponentially with a decrease in r. From the asymptote of Eq. (1) for $r \to \infty$, we obtain:

$$a_{0,quas} = \sqrt{\frac{2m\alpha}{\hbar^2}}\left(1 + \frac{\hbar b}{\sqrt{32m\alpha}}\right) \tag{2}$$

In the same way, for a potential with the asymptote

$$U(r) = \frac{\alpha}{r^4}\left(1 + \frac{b_1}{r} + \frac{b_2}{r^2} + \ldots\right)$$

we can find a more accurate quasi-classical correction to Eq. (2) if we note that, within the required accuracy, it can be written in the form:

$$U = \frac{\alpha}{\left[(r+b)^2 + R^2\right]^2}, \quad \text{where } b = -\frac{1}{4}b_1, \quad R^2 = \frac{5}{16}b_1^2 - \frac{1}{2}b_2$$

For such a potential, the solution of the Schrdinger equation with $E = 0$ can be obtained as in Problem 4.25, and then we find the following correction to Eq. (2):

$$a_{0,quas} = \sqrt{\frac{2m\alpha}{\hbar^2}}\left[1 + \frac{\hbar b_1}{\sqrt{32m\alpha}} + \frac{\hbar^2}{64m\alpha}\left(8b_2 - 5b_1^2\right)\right] \tag{3}$$

The inclusion of these quasi-classical corrections greatly increases the accuracy of the results. For example, according to Eq. (3) instead of the values given in the table in the previous problem, we now have $0.786, 1.002, 1.0005, 1.0001$ in case a, and $0, 0.931,\ 0.999, 0.99998$ in case b.

In conclusion, we give quasi-classical expressions for the scattering length, a_0, in the case of repulsive potentials with other asymptotic behaviors at infinity, $r \to \infty$.

In the case of a power-law asymptote, $U = (\alpha/r^\nu)(1 + b/r + \ldots)$ with $\nu > 3$, we find:

$$a_{0,\text{ quas}} = \frac{\Gamma[(\nu-3)/(\nu-2)]}{\Gamma[((\nu-1)/(\nu-2))]}\left(\frac{2m\alpha}{(\nu-2)^2\hbar^2}\right)^{1/(\nu-2)} + \frac{b}{\nu} \tag{4}$$

where $\Gamma(z)$ is the Γ-function. For $\nu \to 3, a_{0,\text{ quas}} \to \infty$, which reflects the fact that in the potential $U = \alpha/r^3$, the particle scattering cross-section diverges in the limit $E \to 0$.

For a potential with the exponential decrease, $U \approx U_0 e^{-r/R}$,

$$a_{0,\text{ quas}} = R\left[\ln\left(\frac{2mU_0R^2}{\hbar^2}\right) + 2\gamma\right] \tag{5}$$

where $\gamma = 0.5772\ldots$ is Euler's constant.

GKKG.13.35

For an attractive potential, $U(r) \le 0$, that has a power-law decrease, $U \approx -\alpha/r^\nu$ with $\nu > 3$, at large distances, find the scattering length, a_0, in the quasi-classical approximation. Assume that the potential has the following behavior at small distances, $U \propto r^{-\beta}$ with $0 \le \beta < 2$. What is special about the parameters of the potential that correspond to a divergent scattering length?

Consider applications of this result to the potentials a) $U = -\alpha(r + R)^{-4}$, and b) $U = -\alpha\left(r^2 + R^2\right)^{-2}$, and compare to the exact solution.

Solution

At finite distances, the quasi-classical solution of the Schrdinger Eq. (IV.5) for $E = 0$ and $l = 0$ has the form (compare to Problem 9.9):

$$\chi_{\text{quas}} = rR(r) = \frac{C}{\sqrt{p(r)}} \sin\left(\frac{1}{\hbar}\int_0^r p(r)dr + \gamma_0\right), \quad p = \sqrt{-2mU(r)} \tag{1}$$

where γ_0 depends on the form of the potential at small distances. In the case $U \approx -A/r^\beta$ for $r \to 0$, we have:

$$\gamma_0 = -\frac{\pi\beta}{4(2-\beta)}$$

At large distances, $p(r) \to 0$ and the quasi-classical method is not applicable. Here, though, by taking into account the form of potential, $U \approx -\alpha/r^\nu$, we could find the exact solution of the Schrdinger equation:

$$\chi = \sqrt{r}\left[C_1 J_s\left(2s\sqrt{\tilde{\alpha}}r^{-1/2s}\right) + C_2 J_{-s}\left(2s\sqrt{\tilde{\alpha}}r^{-1/2s}\right)\right] \tag{2}$$

where $s = 1/(\nu-2)$ and $\tilde{\alpha} = 2m\alpha/\hbar^2$. On the other hand at distances, where the argument of the Bessel functions in Eq. (2) is large, the quasi-classical approximation is applicable, and both Eqs. (1) and (2) are valid. Using the asymptote of the Bessel function, $J_\nu(z)$, for $z \to \infty$, solution (2) is transformed to

$$\chi = \sqrt{\frac{\pi s\hbar}{p(r)}}\left[C_1 \sin\left(\frac{1}{\hbar}\int_r^\infty pdr - \frac{\pi s}{2} + \frac{\pi}{4}\right) + C_2 \sin\left(\frac{1}{\hbar}\int_r^\infty pdr + \frac{\pi s}{2} + \frac{\pi}{4}\right)\right] \tag{3}$$

We use $p(r) = \sqrt{2m\alpha/r^\nu}$, and by matching Eqs. (3) and (1) obtain:

$$\frac{C_1}{C_2} = -\frac{\sin(\tau + \pi s/2 + \pi/4)}{\sin(\tau - \pi s/2 + \pi/4)}, \quad \tau = \frac{1}{\hbar}\int_0^\infty \sqrt{-2mU(r)}dr + \gamma_0 \tag{4}$$

Furthermore, using an expansion of $J_{\pm s}(z)$ for $z \to 0$, we find the asymptote of solution (2) at large distances:

$$\chi(r) \approx \frac{C_1}{\Gamma(1+s)}(s\sqrt{\tilde{\alpha}})^s + \frac{C_2}{\Gamma(1-s)}(s\sqrt{\tilde{\alpha}})^{-s}, \quad r \to \infty \tag{5}$$

Since $\chi \propto r - a_0$, and taking into account relation (4), we obtain the quasi-classical scattering amplitude as follows:

$$a^{(0)}_{0,quas} \approx \frac{\Gamma(1-s)}{\Gamma(1+s)}\frac{\sin(\tau + \pi s/2 + \pi/4)}{\sin(\tau - \pi s/2 + \pi/4)}\left(s\sqrt{\frac{2m\alpha}{\hbar^2}}\right)^{2s} \tag{6}$$

The parameters of the potential for which the scattering length becomes infinite correspond to the appearance of a new discrete state, as the well becomes deeper. According to Eqs. (6) and (4), this happens when the following conditions are fulfilled (with $l = 0$):

$$\frac{1}{\hbar}\int_0^\infty \sqrt{-2mU(r)}dr = \pi\left[N + \frac{\beta}{4(2-\beta)} + \frac{1}{2(\nu-2)} - \frac{1}{4}\right] \tag{7}$$

where $N = 1, 2, \ldots$ is the sequence number of the new bound state (compare to Problem 9.9).

For the potentials given in the problem condition, we have $\nu = 4, s = 1/2, \gamma = \beta = 0$. From Eq. (6), we obtain

$$\text{a) } a^{(0)}_{0,quas} = R\xi\cot\xi, \text{ b) } a^{(0)}_{0,quas} = R\xi\cot\left(\frac{\pi}{2}\xi\right) \tag{8}$$

where $\xi = \sqrt{\tilde{\alpha}}/R$. The exact values of the scattering length are equal to, respectively, [344]

$$\text{a) } a_0 = R(\xi\cot\xi - 1), \text{ b) } a_0 = R\sqrt{\xi^2+1}\cot\left(\pi\frac{\sqrt{\xi^2+1}}{2}\right) \tag{9}$$

As is seen, for $\xi \to \infty$ the quasi-classical and exact expressions for the scattering length coincide. Their difference scales as $1/\xi$ for finite values of ξ, and is due to quasi-classical corrections. A calculation of such corrections is more difficult (compare to Problem 13.34), since it is necessary to take into account the next term in $\hbar$ in the phase of the wavefunction at finite distances, i.e., in the quasi-classical region.

17.4.2 Problems about low-energy scattering and resonant scattering 2

GKKG.13.36

Consider a quantum particle moving in the presence of two potentials: a long-range potential, $U_L(r)$, with the radius r_L and a short-range potential, $U_S(r)$, with the radius, $r_S \ll r_L$. Treat the latter short-range potential as a small perturbation and generalize the results of Problem 11.4 for the level shift due to $U_S(r)$ (perturbation theory in terms of the scattering length) for a state with an arbitrary angular momentum, l (as opposed to $l = 0$ in Problem 11.4). Assume that at small distances, $r \lesssim r_S$, the long-range potential is weak $\left(|U_L| \ll \hbar^2/mr_S^2\right)$ and that

$$\left|E_{n_r l}^{(0)}\right| \ll \frac{\hbar^2}{mr_S^2}$$

Solution

We use the method described in Problem 11.4. Using ordinary perturbation theory for the potential $U_S(r)$, we obtain

$$\Delta E_{n_r l} = \overline{U_S(r)} = \int U_S(r) \left|\psi_{n_r lm}^{(0)}(\mathbf{r})\right|^2 dV \tag{1}$$

At the relevant small distances (where the potential, $U_S(r)$, has an effect), we can use the following expression for the unperturbed wavefunction:

$$\psi_{n_r lm}^{(0)}(\mathbf{r}) = R_{n_r l}(r) Y_{lm}(\mathbf{n}), \quad R_{n_r l}(r) \approx Q_{n_r l} r^l \quad \text{for } r \ll r_L$$

Using this, we can express integral (1) in terms of the scattering length with the angular momentum l for the potential $U_S(r)$, in the Born approximation (see Problem 13.28):

$$a_l^B = \frac{\pi m}{2^{2l+1}\Gamma^2(l+3/2)\hbar^2} \int_0^\infty r^{2l+2} U_S(r) dr$$

Finally, by replacing a_l^B with the exact scattering length, a_l^S, in the short-range potential, $U_S(r)$, we obtain the level shift expressed in terms of the scattering length:

$$\Delta E_{n_r l} = \frac{\hbar^2}{2m}[(2l+1)!!]^2 Q_{n_r l}^2 a_l^{(S)} \tag{2}$$

We used the fact that $2^{l+1}\Gamma(l+3/2) = \sqrt{\pi}(2l+1)$!!. Also, note a simplification that occurs for the s-states: $Q_{n0}^2 = 4\pi\psi_{n0}^{(2)}(0)$.

We now discuss the main result - Eq. (2).

1. Since, generally speaking, $a_l^{(S)} \propto r_S^{2l+1}$ while $Q_{n_r l}^2 \propto r_L^{-2l-1}$, then with an increase of l, level shifts decrease fast, $\propto (r_S/r_L)^{2l+1}$. This is connected to a decrease in the penetrability of the centrifugal barrier that divides the regions, where the shortrange and long-range potentials act.

2. If the short-range interaction gives rise to inelastic processes (for example, annihilation into pions due to nuclear interaction for the $p\bar{p}$-hadron atom; see also Problem 11.74), then the scattering length, $a_l^{(S)}$, acquires an imaginary part. In this case, $\Delta E_{n_r l}$ describes not only a shift in energy, but also a widening of the level. The level becomes quasi-stationary and has a finite lifetime.

Let us note that the level width

$$\Gamma_{n_r l} = -2\,\mathrm{Im}\,\Delta E_{n_r l} \propto \mathrm{Im}\, a_l^{(S)}$$

is connected with the inelastic scattering cross-section (the reaction cross-section), $\sigma_{rl}^{(S)}$, in the partial wave with the angular momentum, l due to the short-range interaction of slow particles, since

$$-\operatorname{Im} a_l^{(S)} = \left.\frac{\sigma_{rl}^{(S)}(k)}{4}(2l+1)\pi k^{2l-1}\right|_{k\to 0} \tag{3}$$

Note that the long-range potential can also strongly affect the reaction cross-section for slow particles (see the following problem).

3) As mentioned in Problem 11.4, for the case of angular momentum $l = 0$, if the condition $\left|a_0^{(S)}\right| \ll r_L$ is broken, then Eq. (2) is not applicable. In this case, large shifts of the s-levels are possible in the long-range potential, i.e., a reconstruction of the spectrum occurs (see also Problem 9.3). In the case of $l \neq 0$ we have a different situation and there are no large level shifts, which is due to a low-transparency of the centrifugal barrier. But in the case of a large scattering length, $\left|a_l^{(S)}\right| \gg r_S^{2l+1}$, when there is a shallow level with the angular momentum l in the potential, Eq. (2) does require modification. Here, we note that the solution of the Schrdinger equation in the potential $U_S(r)$ for slow particles, $kr_S \ll 1$, and for the distances $r_s \ll r \ll \left(k^{-1}, r_L\right)$, has the form:

$$R_{kl} \approx C\left[r^l + B_l(k)\frac{1}{r^{l+1}}\right] \tag{4}$$

where

$$B_l^{-1} = \frac{1}{(2l-1)!!(2l+1)!!}k^{2l+1}\cot\delta_l^{(S)}(k)$$

The substitution $k^{2l+1}\cot\delta_l^{(S)} \to -1/a_l^{(S)}$, which leads to Eq. (2) for the level shift (it could be more formally obtained, as in Problem 11.4 for the angular momentum $l = 0$), corresponds to the non-resonant case, where $a_l^{(S)} \leq r_S^{2l+1}$. A generalization of this equation to the resonant case, with the effective range expansion (XIII.15) taken into account, is obtained by replacing $a_l^{(S)}$ with [345]

$$a_l^{(S)} \to \left[\frac{1}{a_l^{(S)}} - r_l^{(S)}E\right]^{-1} \tag{5}$$

Generally speaking, we can put $E = E_{n_r l}^{(0)}$. For $l \neq 0$, the second, singular term in Eq. (4) (which is independent of $a_l^{(S)}$ and scales $\propto 1/r^{l+1}$) is small in the region $r \sim r_L$. This ensures the validity of Eqs. (2) and (5) and yields the corresponding modification of the expression for level shift,

$$\Delta E_{n_r l} = \frac{1}{2}[(2l+1)!!]^2 Q_{n_r l}^2\left(\frac{1}{a_l^{(S)}} - r_l^{(S)}E_{n_r l}^{(0)}\right)^{-1} \tag{6}$$

The importance of the $l \neq 0$ condition to the validity of Eq. (6) in the resonant case is connected to a large effective radius that makes the level shifts small, since

[345] Below in this footnote $\hbar = m = 1$, so that $E = k^2/2$. Note that Eq. (4) can be viewed as a boundary condition for the Schrdinger equation with potential $U_L(r)$ at small distances, which is due to the appearance of the short-range potential $U_S(r)$ (compare to Problem 11.4). But in the case $l \neq 0$, to take the limit $r \to 0$ is impossible due to the divergence of the normalization integral (since it gives $\psi \propto 1/r^{l+1}$ at short distances $r \leq r_s$, the wavefunction coincides with that in the short-range potential). In the case $l = 0$, the limit $r_s = 0$ is possible and corresponds to approximating of the short-range potential by a zero-range potential. See Problem 4.10.

$r_l^{(S)} \propto r_S^{1-2l}$ (see Problem 13.44). The substitution $E = E_{n_r l}^{(0)}$ used in Eqs. (5) and (6) is invalid only if

$$E_S^{(0)} \equiv \frac{1}{a_l^{(S)}}r_l^{(S)} \approx E_{n_r l}^{(0)} \tag{7}$$

This is because $E_S^{(0)}$ describes a level with the angular momentum l that exists in an isolated potential, $U_S(r)$. Condition (7) is fulfilled when there are two close levels, related to both potentials. If we do not substitute $E_{n_r l}^{(0)}$ for E in Eq. (6), we obtain a equation for $\Delta E_{n_r l} = E - E_{n_r l}^{(0)}$, and solve it as follows:

$$E_{1,2} = \frac{1}{2}\left\{E_S^{(0)} + E_{n_r l}^{(0)} \pm \left[\left(E_S^{(0)} - E_{n_r l}^{(0)}\right)^2 + \frac{1}{\left|r_l^{(S)}\right|}((2l+1)!!)^2 Q_{n_r l}^2\right]^{1/2}\right\} \tag{8}$$

This gives the energy of these levels with their interaction taken into account. Note that this equation describes "quasi-crossing" levels. In the case of $E_S^{(0)} > E_{n_r l}^{(0)}$, one of the roots of Eq. (8) describes a shift of the unperturbed level $E_S^{(0)}$ upwards under the influence of the long-range potential, [346] $U_L(r)$, while the second

one describes a level shift downward of $E_{n_r l}^{(0)}$ under the influence of the short-range potential, $U_S(r)$. In the case $E_S^{(0)} < E_{n_r l}^{(0)}$, their roles are switched.
Finally, we discuss the form of wavefunctions in the presence of a level quasicrossing. For a sufficiently large difference between $E_S^{(0)}$ and $E_{n_r l}^{(0)}$, with $E_S^{(0)} > E_{n_r l}^{(0)}$, the wavefunction that corresponds to the first of the levels in Eq. (8) is approximately $\psi_S^{(0)}$, localized at small distances $r \lesssim r_s$, while the wavefunction that corresponds to the second level in Eq. (8) is approximately $\psi_{n_r l}^{(0)}$ localized at large distances, $r \sim r_L$. In the case $E_S^{(0)} < E_{n_r l}^{(0)}$, wavefunctions corresponding to the two levels (in the essential localization domain) change places. In the case of an exact resonance $E_S^{(0)} = E_{n_r l}^{(0)}$, the quantum particle occurs in the two states with an equal probability (equal to 1/2); i.e., has the same probability, 1/2, to be bound in either the localization domains of the potential $U_S(r)$ (for $r \lesssim r_S$) and or that of $U_L(r)$ (for $r \sim r_L$). Wavefunctions of the corresponding states are the same for $r \lesssim r_s$ and differ by a sign in the region $r \gg r_s$, which gives rise to their orthogonality.

[346] Strictly speaking, here we reproduce only the part of the shift that is connected to the action of $U_L(r)$ at large distances, $r \gg r_s$. The influence of U_L on the level shift $E_S^{(0)}$ at short distances manifests itself in a renormalization of the parameters $a_l^{(S)}, r_l^{(S)}$. For example, if $U_L(r) \approx U_0$ for $r \leq r_S$, then it would be more accurate to replace E in Eq. (5) by $E - U_0$. Such a replacement corresponds to a renormalization of the scattering length, i.e., replacing $a^{(S)}$ by $a_l^{(SL)}, 1/a_l^{(SL)} = 1/a_l^{(S)} + r_l^{(S)} U_0$. The effective radius is not renormalized in this case. See also Problem 13.42.

GKKG.13.37

A particle is moving in a combined field of two potentials: a strong short-range potential $U_S(r)$ with the radius r_S and a long-range potential $U_L(r)$ with the radius $r_L \gg r_S$, which is weak at small distances $r \lesssim r_S : |U_L| \ll \hbar^2/m r_S^2$. Assuming that the solution of the Schrdinger equation for the potential $U_L(r)$ is known, find a change of the phase shift, $\Delta\delta_l^{(S)}$, in this potential under the influence of U_S, in the case of slow particles, so that $kr_S \ll 1$. Express $\Delta\delta_l^{(S)}$ in terms of the scattering length $a_l^{(S)}$ in the potential U_S.
Under what conditions is the phase shift in the field $U = U_S + U_L$ approximately equal to the sum of phase shifts in the potentials U_S and U_L separately?
Apply this result to the long-range Coulomb potential.

Solution

We are going to use the methods developed in the previous problem: (1) find a change of the phase shift, $\Delta\delta_l^{(S)}$, by perturbation theory, (2) express it in terms of the scattering length by a short-range potential in the Born approximation, and (3) replace the scattering length by the exact scattering length $a_l^{(S)}$ in the "strong" potential $U_S(r)$. A formal justification of this method is provided in Problem 11.4.

To determine the shift, $\Delta\delta_l^{(S)}$, under the influence of $U_S(r)$ by perturbation theory, we write two Schrdinger equations for the radial wavefunctions, $\psi_{klm} = \chi_{kl} Y_{lm}/r$, of the continuous spectrum:

$$\begin{aligned} \chi_{kl}^{(0)''} + \left[k^2 - \frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2} U_L(r)\right] \chi_{kl}^{(0)} = 0 \\ \chi_{kl}'' + \left[k^2 - \frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2} \left(U_L(r) + U_S(r)\right)\right] \chi_{kl} = 0 \end{aligned} \tag{1}$$

The solutions of these equations, which correspond to the boundary condition $\chi(0) = 0$, have the following asymptotes at large distances:

$$\begin{aligned} \chi_{kl}^{(0)} \approx \sin\left(kr \pm \frac{Z}{k a_B} \ln 2kr - \frac{\pi}{2} l + \delta_l^{(L)}\right) \\ \chi_{kl} \approx \sin\left(kr \pm \frac{Z}{k a_B} \ln 2kr - \frac{\pi}{2} l + \delta_l^{(L)} + \Delta\delta_l^{(S)}\right) \end{aligned} \tag{2}$$

For concreteness, we have considered the case where at large distances: $U_L \approx \mp Z e^2/r$, $a_B = \hbar^2/me^2$.

Multiplying the first of the equations in (1) by χ_{kl} and the second by $\chi_{kl}^{(0)}$, subtracting them term by term, and integrating over r from 0 to ∞, we obtain:

$$k \sin \Delta\delta_l^{(S)} = -\frac{2m}{\hbar^2} \int_0^\infty U_S(r) \chi_{kl}(r) \chi_{kl}^{(0)}(r) dr \tag{3}$$

We can approximate the sine-function by its argument, and χ_{kl} by $\chi_{kl}^{(0)}$. Taking into account the short-range nature of the potential U_S and also the relation $\chi_{kl}^{(0)} \approx Q_{kl} r^{l+1}$ for $r \to 0$, we find:

$$\Delta\delta_l^{(S)} = -\frac{2m}{\hbar^2 k} Q_{kl}^2 \int_0^\infty r^{2l+2} U_S(r) dr \tag{4}$$

The integral here is expressed in terms of the scattering length with angular momentum l in the Born approximation (see the previous problem). Now, we replace it by the exact scattering length, and obtain the desired result:

$$\Delta\delta_l^{(S)}(k) = -[(2l+1)!!]^2 a_l^{(S)} \frac{Q_{kl}^2}{k} \tag{5}$$

We now analyze Eq. (5):

1. Let us first note that in the case $U_L \equiv 0$, we have

$$\chi_{kl}^{(0)} = \sqrt{\frac{\pi k r}{2}} J_{l+1/2}(kr)$$

Here,

$$Q_{kl}^2 = \frac{k^{2l+2}}{[(2l+1)!!]^2}$$

so that

$$\Delta\delta_l^{(S)} = -a_l^{(S)} k^{2l+1} \tag{6}$$

i.e., Eq. (6) coincides with the scattering phase $\delta_l^{(S)}$ from the isolated potential $U_S(r)$, as it should be.
2) The same relation, $\Delta\delta_l^{(S)} = \delta_l^{(S)}$, holds approximately also in the case of a longrange potential $U_L(r)$ that can be considered as perturbation (see conditions (XIII.7)). In this case, the scattering phase in the potential, which is the superposition $U_S(r) + U_L(r)$, is equal to the sum of the scattering phases for each of them separately.
3) Let us finally focus on the case of the long-range Coulomb potential, $U_L = \mp Ze^2/r$. Here,

$$\chi_{kl}^{(0)} = \frac{Zr}{a_B} C_{kl}^{(\mp)} \frac{(2kr)^l}{(2l+1)!} e^{\mp ikr} F\left(i\frac{Z}{ka_B} + l + 1, 2l+2, \pm 2ikr\right)$$

$$\delta_l^{(L)} = \arg \Gamma\left(l + 1 \mp \frac{iZ}{ka_B}\right)$$

$$C_{kl}^{(\mp)} = 2k' e^{\pm\pi/2k'} \left|\Gamma\left(l + 1 \mp \frac{i}{k'}\right)\right| =$$

$$e^{\pm\pi/2k'} \left(\frac{\pi k'}{\sinh \pi k'}\right)^{1/2} \prod_{s=1}^{l} \sqrt{s^2 + \frac{1}{(k')^2}}$$

We let $k' = ka_B/Z$, so that

$$\left(Q_{kl}^{(\mp)}\right)^2 = \frac{\pi Z (2k)^{2l+1}}{[(2l+1)!]^2 a_B} \frac{(\mp 1)}{e^{\mp 2\pi Z/ka_B} - 1} \prod_{s=1}^{l} \left[s^2 + \left(\frac{Z}{ka_B}\right)^2\right] \tag{7}$$

For $l = 0$, the products are replaced by 1.
In the case of "fast" particles, when $ka_B \gg Z$ (but still $kr_s \ll 1$), the Coulomb potential could be considered as a perturbation, and from Eqs. (5) and (7), the results discussed above in 1) and 2) follow.

A completely different situation arises for $ka_B \le Z$. Here, values of $Q_{kl}^{(\mp)}$ differ greatly from the unperturbed values given in 1). Particularly for $ka_B \ll Z$, according to Eqs. (5) and (7), for an s-wave we obtain

$$\text{a) } \Delta\delta_0^{(S)} = \frac{2\pi Z}{ka_B} \delta_0^{(S)}; \quad \text{b) } \Delta\delta_0^{(S)} = \frac{2\pi Z}{ka_B} e^{-2\pi Z/ka_B} \delta_0^{(S)} \tag{8}$$

for the attractive and repulsive Coulomb potential respectively. The essential change of the phase shift value (its increase by $2\pi Z/ka_B \gg 1$ in the case of attraction, and its exponential decrease in the case of repulsion)

has a clear physical underpinning: in the case of slow particles the long-range Coulomb attraction (repulsion) greatly increases (decreases) the probability of finding particles at small distances. This also strongly affects the cross-sections of inelastic processes caused by a short-range interaction, that accompany collisions of slow particles.

In conclusion, let us note that all of this assumes that the scattering from the short-range potential is non-resonant, i.e., there is no "shallow" level in the potential $U_S(r)$. Here $a_l^{(S)} \leq r_S^{2l+1}$ and $\delta_l^{(S)} \approx -a_l^{(S)} k^{2l+1} \ll 1$. However, by substituting the scattering length $a_l^{(S)}$, as in the previous problem, with the expression

$$\left(\frac{1}{a_l^{(S)}} - \frac{1}{2} k^2 r_l^{(S)} \right)^{-1} \tag{9}$$

Eq. (5) could be generalized to include the resonant case. The condition of its applicability is $\Delta\delta_l^{(S)} \ll 1$ (which was used to transform Eq. (3)). Note that for
a repulsive long-range potential, this condition may remain satisfied even if the scattering phase $\delta_l^{(S)}$ for the isolated short-range potential $U_S(r)$ is not small. [347]

GKKG.13.38

How should we modify the Rutherford formula to describe the differential scattering cross-section in the Coulomb potential $U = \pm Ze^2/r$, which is "distorted" at small distances $r \lesssim r_S$? Assume that the conditions $kr_S \ll 1$ and $Ze^2 \ll \hbar v$ are fulfilled. The distortion of the Coulomb field is described by a potential $U_S(r)$, with a known scattering length, $a_0^{(S)}$.

Solution

The scattering amplitude is described by the expression:

$$f \approx f_{\text{Coul}} + f_S; \quad f_{\text{Coul}} = \pm \frac{Ze^2 m}{2\hbar^2 k^2 \sin^2(\theta/2)}, \quad f_S = -a_0^{(S)} \tag{1}$$

This follows from the fact that we only need to consider influence of the short-range potential, $U_S(r)$, on the particles with the angular momentum $l = 0$ (since $kr_s \ll 1$), and that we can consider the Coulomb potential as a perturbation (since $Ze^2 \ll \hbar v$). According to the previous problem, the phase shift in the total potential field (the superposition $U_{\text{Coul}} + U_S$) is approximately equal to the sum of phase shifts for each of the potentials separately.

The differential scattering cross-section is described by

$$\frac{d\sigma}{d\Omega} = \left(\frac{Ze^2}{2mv^2} \right)^2 \frac{1}{\sin^4(\theta/2)} + \left(a_0^{(S)} \right)^2 \mp \frac{Ze^2 a_0^{(S)}}{mv^2 \sin^2(\theta/2)} \tag{2}$$

The last term corresponds to an interference of the scattering amplitudes due to the Coulomb and the short-range interactions. As is seen, its character depends of the sign of the scattering length $a_0^{(S)}$.

GKKG.13.39

Find the scattering length, a_l, of a particle with an arbitrary angular momentum, l for the following potentials:
a) an impenetrable sphere with radius R;
b) $U(r) = -\alpha\delta(r - R)$
c) a square well of radius R and depth U_0.

Compare to the case of $l = 0$ from Problem 13.31.

[347] However, if the scattering length is large, a renormalization of the parameters describing low-energy scattering may become significant. See the previous problem, and also Problem 13.42.

Solution

The scattering length, a_l, could be found from the asymptote of the radial wavefunction, $R_{kl}(r)$, for $E = 0$:

$$R_{0l} \approx r^l - \frac{1}{r^{l+1}} \left\{ (2l-1)!!(2l+1)!! a_l \right\}, \text{ for } r \to \infty$$

This follows, for example, from a comparison of the expression for the wavefunctions of slow particles at distances $d \ll r \ll 1/k$:

$$R_{kl} \approx r^l + B_l(k)\frac{1}{r^{l+1}}, \quad B_l^{-1} = \frac{k^{2l+1}\cot\delta_l}{(2l-1)!!(2l+1)!!}$$

with the effective range expansion (XIII.15).
Below, we present the final results:
a) for scattering from the impenetrable sphere:

$$a_l = \frac{1}{(2l-1)!!(2l+1)!!}R^{2l+1} \equiv a_{sph,l} \tag{1}$$

b) for scattering from the δ-well:

$$a_l = \frac{\xi}{\xi - 2l - 1}a_{sph,l}, \quad \xi = \frac{2m\alpha R}{\hbar^2} \tag{2}$$

c) for scattering from the square potential well:

$$a_l = -\frac{J_{l+3/2}(\lambda)}{J_{l-1/2}(\lambda)}a_{sph,l}, \quad \lambda = \sqrt{\frac{2mU_0R^2}{\hbar^2}} \tag{3}$$

Note that the properties of the scattering length, a_l, as a function of the parameters of the potentials (in cases *b*) and *c*)) are similar to those considered in Problem 13.31 for an s-wave. In particular, when a new bound state appears, the scattering length, a_l, becomes infinite.

GKKG.13.40

Estimate the singlet (i.e., the total electron spin is $S = 0$) electron s-scattering length, $a_0(1)$, for scattering off of an unexcited hydrogen atom. Keep in mind that there exists a weakly-bound state, the ion H^-, with the binding energy $\varepsilon_0 = 0.754\text{eV} = 0.0277$ a.u.
a) Neglect the finite-size effects for both the atomic size and the interaction range of the external electron with the atom.
b) Consider the external electron as weakly bound in a finite-range potential, and use the following asymptotic coefficient $C_{\kappa 0}^2 = 2.65$ (see Problem 11.36).
Compare to the result of a variational calculation: $a_0(1) = 5.97$ a.u.

Solution

a) In this approximation, which corresponds to considering the external electron as in a zero-range potential, we have (see Problems 13.20 and 4.10):

$$a_0 = \kappa_0^{-1} = (2\varepsilon_0)^{-1/2} = 4.25 \tag{1}$$

(in atomic units).
b) Considering the external electron as weakly bound in the potential of finite radius r_S, we first use the relation between the effective interaction radius r_0 and the asymptotic coefficient:

$$r_0 = \frac{C_{\kappa 0}^2 - 1}{\kappa_0 C_{\kappa 0}^2}$$

Now, taking into account the effective-range expansion, Eq. (XIII.15), and the fact that the scattering amplitude, as a function of energy, has a pole at $E = -\varepsilon_0$ (Note that at the pole, $k\cot\delta_0 = ik = -\kappa_0$), we find:

$$a_0 = \frac{2C_{\kappa 0}^2}{\kappa_0\left(1 + C_{\kappa 0}^2\right)} = 6.17 \tag{2}$$

As is seen, the correction to the effective radius strongly affects the value of the scattering length. This is because $\kappa_0 r_s \approx 0.6$ is not that small. In connection to this, let us mention the role of the subleading, $\propto k^4$, term in the effective-range expansion, Eq. (XIII.15). It is usually written as

$$-Pr_0^3k^4 \tag{3}$$

A typical value of this parameter, P, here is small, $|P| \lesssim 0.1$. Taking this into account, we should see that the scattering length (2) is determined to within a few percent accuracy.

GKKG.13.41

In a proton-neutron system, estimate the triplet s-wave scattering length, $a_0(3)$, taking into account the existence of a weakly bound state, the deuteron, with the binding energy $\varepsilon_0 = 2.23\text{MeV}$. Compare to the experimental value, $a_0(3) = 5.39 \cdot 10^{-13}$ cm.

Solution

Neglecting the finiteness of the effective range of the interaction, we have

$$a_0(3) = \kappa_0^{-1} = \left(\frac{\hbar^2}{2\mu\varepsilon_0}\right)^{1/2} = 4.3 \cdot 10^{-13} \text{ cm} \tag{1}$$

where $\mu \approx m_p/2$ is the reduced mass of the pn-system. Since the range of the nuclear forces is $r_s \sim 10^{-13}$ cm, then $\kappa_0 r_s \sim 0.3$, Equation (1) has the same accuracy: about 20%. If we include the term with the effective range $\left(r_0(3) = 1.7 \cdot 10^{-13} \text{ cm}\right)$ in
expansion (XIII.15), we reproduce the experimental value of the triplet scattering length. Compare with the previous problem.

GKKG.13.42

a) Using the experimental value of the singlet s-wave scattering length, $a_0(1) = -23.7 \cdot 10^{-13}$ cm, for a proton-neutron system, estimate the energy of the shallow virtual level [348] in such a system in the state with $S = 0$ and $l = 0$.
b) For a proton-proton system, $a_0(1) = -7.77 \cdot 10^{-13}$ cm. Does the significant difference between the scattering lengths for the pn - and pp-systems contradict the isotopic invariance of the nuclear interaction? The effective range of the interaction $r_0(1)$, is equal to $2.67 \cdot 10^{-13}$ cm and $2.77 \cdot 10^{-13}$ cm, respectively, for the pn - and pp-systems.

Solution

a) Neglecting the effective range of the interaction, we obtain (compare to Problems 13.20 and 4.10, and also Problem 13.40)

$$\varepsilon_{virt} \approx \frac{\hbar^2}{2\mu a_0^2(1)} = 56\text{keV}$$

Here, $\mu = m_p/2$ is the reduced mass of the pn-system.
b) Since the Coulomb interaction at small distances is weaker than the nuclear forces by approximately two orders of magnitude, then navely we might assume that the difference of the low-energy scattering parameters for the pp-system from those for the pn-system should remain to within a few percent. This is indeed so specifically for the effective range of the interaction.

The scattering lengths however do differ noticeably: by a factor of three. But this does not imply that isotopic invariance of nuclear interactions is strongly broken, since the difference could be explained by the Coulomb interaction in the pp-system. In the pn-system there is a shallow virtual level, and the scattering length is large (approximately twenty times larger than the interaction radius!). In such conditions, this function depends sharply on the parameters of the potential (see Problem 13.31), and differs greatly for even a small change of those (in this problem, due to the Coulomb interaction).

Let us provide a simple estimate of the renormalization of the scattering length. We write the pn-interaction in the form $U_{pn} = U_0(r) + \delta U(r)$, where $U_0(r)$ corresponds to the threshold of the appearance of a new bound state, here $\delta U(r) \geq 0$, since the level in the pn-system is virtual. For the pp-system, considering protons to be point-like, we have $U_{pp} = U_0 + \delta U + e^2/r$. Using the result of Problem 4.27 for a shallow s-level depth, we find:

$$\kappa_{pp} = -\frac{2\mu}{\hbar^2} \int_0^d \left(\delta U(r) + \frac{e^2}{r}\right) \chi_0^2(r) dr \tag{1}$$

We use $\chi_0(r)$ as the wavefunction ($\chi = rR$) at the threshold of the appearance of a new bound state, normalized by the condition $\chi_0(r) = 1$ outside of the potential range. The upper integration limit is $d \sim a_B = \hbar^2/m_p e^2 \approx 29 \cdot 10^{-13}$ cm. (At larger distances, a contribution coming from the Coulomb interaction is taken into account independently, and appears in the amplitude of Coulomb scattering of the protons.) The integral of $\delta U(r)$ in Eq. (1) gives κ_{pn} (in both systems $\kappa < 0$, since the levels are virtual). To estimate the integral of the Coulomb potential, we put $\chi_0^2(r) = 1$. Due to a divergence in the lower limit, we introduce a cutoff at $r_s \approx 10^{-13}$ cm (of the order of the nuclear interaction radius). Finally, taking into account the relations $\kappa_{pn} = 1/a_0^{pn}(1)$ and $\kappa_{pp} = 1/a_0^{pp}(1)$, according to Eq. (1), we obtain:

$$\frac{1}{a_0^{pp}(1)} - \frac{1}{a_0^{pn}(1)} \approx -\frac{1}{a_B} \ln\left(\frac{a_B}{r_0}\right) \tag{2}$$

Here, instead of r_s, we put the effective interaction radius, r_0. Let us emphasize that the uncertainty in parameters d and r_s, for which $d/r_s \gg 1$, is "softened" in the final result because of the logarithm. So, we see that accounting for the protons' "weak" Coulomb interaction explains the significant difference of the scattering lengths for the pp - and pn-systems.

GKKG.13.43

Prove the following relation for the effective range of the interaction (see, Eq. (XIII.15)):

$$r_0 = 2\int_0^\infty \left\{\left(-\frac{r}{a_0}+1\right)^2 - \chi_0^2(r)\right\} dr$$

where $\chi_0(r)$ is the radial wavefunction ($\chi_0 = rR_0$) of a state with $l = 0$ and $E = 0$, normalized by the condition $\chi_0(r) = (-r/a_0 + 1)$ for $r \to \infty$ (a_0 is the scattering length).

Find r_0 for an impenetrable sphere of radius R, and also for a δ-well, $U(r) = -\alpha\delta(r - R)$ and a square well of radius R at the threshold for bound state formation ($a_0 = \infty$) in the two latter cases.

Solution

We denote the radial wavefunctions for the values of energy $E = 0$ and $E = \hbar^2k^2/2m$ by χ_0 and χ, respectively. They satisfy the following equations:

$$\chi_0'' - \tilde{U}(r)\chi_0 = 0, \quad \chi'' - \left[\tilde{U}(r) - k^2\right]\chi = 0; \quad \tilde{U} = \frac{2m}{\hbar^2}U(r) \tag{1}$$

To normalize $\chi_0(r)$, use the condition $\chi_0(r) \approx (1 - r/a_0)$ for $r \gg d$ (d is the potential radius). For wavefunction $\chi(r)$ at distances $d \ll r \ll 1/k$, we have

$$\chi(r) = k\cot\delta_0 \cdot r\left[1 + O\left(k^2r^2\right)\right] + \left[1 + O\left(k^2r^2\right)\right] \tag{2}$$

where $O\left(k^2r^2\right)$ corresponds to corrections in the asymptote.

Multiplying the first equation of (1) by χ, the second one by χ_0, subtracting them term by term, and integrating in the region where expansion (2) is valid, we obtain:

$$\int_0^r \frac{d}{dr}\left\{\chi_0'\chi - \chi_0\chi'\right\} dr \equiv -\frac{1}{2}r_0k^2 + O\left(k^2r, k^2\frac{r^2}{a_0}, k^2\frac{r^3}{a_0^2}\right) =$$

$$k^2\int_0^r \chi(r)\chi_0(r)dr \tag{3}$$

Here, we have taken into account the asymptotes given above, the boundary condition $\chi(0) = 0$, and the effective range expansion (XII.15). The integral on the right-hand side of the expression can be cast into the form

$$\int_0^r \chi\chi_0 dr \approx \int_0^r \left[\chi_0^2 \pm \left(-\frac{r}{a_0}+1\right)^2\right] dr =$$

$$= \int_0^r \left[\chi_0^2 - \left(-\frac{r}{a_0}+1\right)^2\right] dr + \frac{r^3}{3a_0^2} - \frac{r^2}{a_0} + r$$

(here we have used $\chi \approx \chi_0$; the notation $\pm(-r/a_0 + 1)^2$ means an addition or subtraction of the corresponding term).

We have used the fact that $\chi \approx \chi_0$. In the last integral we could extend the integration to infinite limits. Then, leaving only r independent terms in Eq. (3), we obtain

$$r_0 = 2\int_0^\infty \left\{\left(-\frac{r}{a_0}+1\right)^2 - \chi_0^2(r)\right\} dr \tag{4}$$

For the scattering from an impenetrable sphere of radius R we have $\chi_0 = 1 - r/R$ for $r > R$ and $\chi_0 = 0$ for $r < R$. In this case, the scattering length is $a_0 = R$, and according to Eq. (4) we find the effective range of the interaction, $r_0 = \frac{2}{3}R$.

For $a_0 = \infty$ from Eq. (4) the well-known result for effective range, r_0, at the threshold of s-level appearance follows. In particular, for the scattering from a δ well with $a_0 = \infty$, we have $\chi_0 = 1$ for $r > R$ and $\chi_0 = r/R$ otherwise. According to Eq. (4) with $a_0 = \infty$, we obtain $r_0 = \frac{4}{3}R$. For the scattering from a square potential well $r_0 = R$, and the effective range is the same whenever a new bound state appears (independently of its sequence number). Here, for $r < R$, the wavefunction is

$$\chi_0 = \sin\left[\pi\left(n_r + \frac{1}{2}\right)\frac{r}{R}\right]$$

where $n_r = 0, 1, 2, ...$ is the sequence number of bound state that appear with a deepening of the well.

Note that both the value $r_0 \sim R$ and the sign $r_0 > 0$ of the "critical" effective range (at the threshold of appearance of a new s-state) are quite general for attractive potentials, $U(r) \leq 0$. Compare to the case of angular momenta $l \neq 0$ in Problem 13.44, and also to the case $l = 0$ for a well surrounded by a potential barrier, in Problem 13.47.

GKKG.13.44

Prove that the effective range of the interaction r_l, in a state with $l \neq 0$ (see Eq. (XIII.15)) and at the threshold of bound-state [349] formation, is

$$r_l = -2[(2l-1)!!]^2 \frac{1}{C_l^2}$$

where C_l is the normalization coefficient in the wavefunction of the zero-energy state ($E = 0$):

$$\chi_l^{(0)}(r) \approx C_l \frac{1}{r^l} \text{ for } r \to \infty \text{ and } \int_0^\infty \left(\chi_l^{(0)}(r)\right)^2 dr = 1$$

Find r_l for a δ-well.

Solution

We will follow the method outlined in the previous problem. Taking into account that the wavefunction when a new bound state is just about to appear has the form $\chi_l^{(0)} = C_l r^{-l}$ for $r \gg d$, and also the relation

$$\chi_{kl} \approx C_l \left[r^{-l} + \frac{k^{2l+1}\cot\delta_l}{(2l-1)!!(2l+1)!!} r^{l+1}\right], \quad d \ll r \ll \frac{1}{k}$$

(compare, for example, to Problem 13.39), we find:

$$-\frac{1}{[(2l-1)!!]^2} C_l^2 k^{2l+1}\cot\delta_l = k^2 \int_0^r \chi_{kl}\chi_l^{(0)}, \quad d \ll r \ll \frac{1}{k}$$

Now, if we replace χ_{kl} by $\chi_l^{(0)}$ in the right-hand side (due to a small value of k^2), extend the integration to infinity (in the case $l = 0$, we cannot do this due to a divergence of

[349] This case is interesting, since in the absence of a shallow level in the potential, the term containing the effective range in Eq. (XIII.15) acts as a small correction.

the integral at the upper limit) and use the relation $k^{2l+1}\cot\delta_l = r_l k^2/2$ (since $a_l = \infty$ at the threshold), then we obtain:

$$r_l = -2[(2l-1)!!]^2 C_l^{-2}, \quad l \geq 1 \tag{1}$$

The value of C_l^2 is uniquely determined by the normalization of the radial wavefunction, $\chi_l^{(0)}$, to 1.

Unlike in the case of s-scattering, the effective range of the interaction is negative, $r_l < 0$, and is of the order of $|r_l| \sim R^{1-2l}$, where R is the radius of the potential (which is of the same magnitude as the localization domain of a zero-energy bound-state with the angular momentum $l \neq 0$).

For a δ-well, the wavefunction at the threshold of appearance of a new bound state with the angular momentum, l, has the form:

$$\chi_l^{(0)} = \begin{cases} C_l r^{-l}, & r > R \\ C_l \frac{r^{l+1}}{R^{2l+1}}, & r < R \end{cases}$$

From the normalization condition, we find C_l^2 and the effective range of the interaction is:

$$r_l = -\frac{4(2l-3)!!(2l+1)!!}{2l+3}R^{1-2l}, \quad l \geq 1$$

In conclusion, note that a change in the effective range as a result of a small change in the potential is also small. So, the "critical" value of r_l at the threshold of bound-state formation is applicable also in the case of a shallow level (real and quasi-discrete).

17.4.3 Problems about low-energy scattering and resonant scattering 3

GKKG.13.45

Find the phase shift, $\delta_0(k)$, and scattering cross-section for scattering of slow particles in the following potentials:
a) an impenetrable sphere of radius R;
b) a δ-well, $U(r) = -\alpha\delta(r-R)$;
c) a square well of radius R and depth U_0.
Use the effective range expansion.

Solution

a) For the radial function $\chi_l = rR_l$ with $l = 0$, the Schrdinger equation and its solution, which corresponds to the boundary condition $\chi_0(R) = 0$, have the form:

$$\chi_0'' + k^2\chi_0 = 0, \quad \chi_0(r) = A\sin[k(r-R)]$$

So, the s-scattering phase shift is $\delta_0(k) = -kR$, and the scattering cross-section for slow particles, when $kR \ll 1$, is described by the expression:

$$\sigma \approx \sigma_{l=0}(k) = \frac{4\pi}{k^2}\sin^2\delta_0 \approx 4\pi R^2\left(1 - \frac{1}{3}k^2R^2\right)$$

Recall that the first correction to the cross-section is connected with p-wave scattering, and is $\propto k^4$. The contribution of higher waves is less important.
In the cases *b*) and *c*), it is also possible to find $\delta_0(k)$ from a exact solution to the Schrdinger equation. But it is easier to consider slow particle scattering using the effective range expansion, Eq. (XIII.15). The parameters of low-energy scattering, a_l and r_l, could be obtained using the zero-energy solution of the Schrdinger equation. See Problems 13.31 and 13.43, specifically for a discussion of the s-wave scattering.
b) The solution of the Schrdinger equation for $E = 0$ and $l = 0$ has the form:

$$\chi_0(r) = \begin{cases} r - a_0, & r > R \\ Cr, & r < R \end{cases}$$

Matching the solution at the point $r = R$ (see Problem 2.6) gives:

$$a_0 = \frac{\tilde{\alpha}R}{\tilde{\alpha}-1}, \quad C = 1 - \frac{a_0}{R}, \quad \tilde{\alpha} = \frac{2m\alpha R}{\hbar^2}$$

If $\tilde{\alpha}$ is not close to 1, then $|a_0| \leq R$, and for slow particles $\sigma \approx 4\pi a_0^2$ (a correction of the order of k^2R^2 to this expression could be found by calculating the effective range, r_0, according to Problem 13.43). However, if $\tilde{\alpha}$ is close to 1, then $|a_0| \gg R$ and the scattering cross-section has a pronounced energy-dependence that is described by resonance equation (XIII.16). For this, the effective range of the interaction for a δ-well at the threshold of s-state formation is $r_0 = \frac{4}{3}R$ (see Problem 13.43). Note that the relation $\sigma \approx 4\pi a_0^2$ needs to be corrected also for values of the parameter $\tilde{\alpha}$ close to $2l+1$ with $l \geq 1$ (when a bound state with the angular momentum l appears in the system), due to the resonant nature of scattering in the l-th partial wave (see Problem 13.46).
c) The parameters of low-energy scattering, a_0 and r_0, for the square potential well were found in Problems 13.31 and 13.43.

GKKG.13.46

Consider scattering of slow particles in the partial wave with the angular momentum, $l \neq 0$, for the potential $U(r) = -\alpha\delta(r-R)$. Consider specifically the case of angular resonant scattering with a quasi-stationary state of small energy, $E_R \ll \hbar^2/mR^2$, and find its width, Γ_R.

Solution

As in the previous problem, we use the effective range expansion, Eq. (XIII.15). The scattering length,

$$a_l = -\frac{1}{(2l-1)!!(2l+1)!!}\frac{\tilde{\alpha}}{2l+1-\tilde{\alpha}}R^{2l+1}, \quad \tilde{\alpha} = \frac{2m\alpha R}{\hbar^2} \tag{1}$$

was calculated in Problem 13.39. When $\tilde{\alpha}$ is not close to $2l+1$, the scattering in l th partial wave is non-resonant. For slow particles,

$$\sigma_l \approx 4\pi(2l+1)a_l^2 k^{4l}$$

and the dominant scattering is s-wave.
If $\tilde{\alpha}$ is close to $2l+1$, then in the potential there exists a shallow real (for $\tilde{\alpha} > 2l+1$) or quasi-discrete [350] (for $\tilde{\alpha} < 2l+1$) level. Scattering has a resonant nature, and the term with the following effective range (according to Problem 13.44)

$$r_l \approx -4(2l-3)!!(2l+1)!!\frac{R^{1-2l}}{2l+3} \tag{2}$$

is essential.
The energy spectrum is determined by the poles of the partial scattering amplitude $f_l(E) = 1/k\,(\cot\delta_l - i)$. At the pole E_l we have $\cot\delta_l(E_l) = i$, and using the effective range expansion, Eq. (XIII.15), we obtain for "shallow" levels:

$$ik_R^{2l+1} = -\frac{1}{a_l} + \frac{1}{2}r_l k_R^2 \tag{3}$$

In the case $l \geq 1$, the left-hand side of this equation is small in comparison to both terms in the right-hand side, so that it could be solved by successive iterations. In the "zeroth" approximation, neglecting the left part in Eq. (3), we obtain:

$$E_R \approx \frac{\hbar^2}{mr_l a_l} \approx \frac{(2l-1)(2l+3)(2l+1-\tilde{\alpha})}{4(2l+1)}\frac{\hbar^2}{mR^2} \tag{4}$$

Since $r_l < 0$ (for $l \geq 1$), then for $a_l > 0$ (i.e., for $\tilde{\alpha} > 2l+1$) we have $E_R < 0$, so that the level corresponds to a bound state in the δ-well (compare to Problem 4.9). For the scattering of slow particles in this case, $f_l \approx (k\cot\delta_l)^{-1}$, while the corresponding partial scattering cross-section is
$$

$$\sigma_l(E) = 4\pi(2l+1)\left|f_l\right|^2 \approx 4\pi(2l+1)\frac{\hbar^4}{m^2 r_l^2}\frac{k^{4l}}{(E+|E_R|)^2} \tag{5}$$

$$
As is seen, $\sigma_l \propto (kR)^{4(l-1)}R^2$, i.e., in this case the resonant cross-section in the l th partial wave has the same order of magnitude as the non-resonant cross-section in the lower partial wave, with the angular momentum equal to $l-1$. So, except for the case $l = 1$, it does not provide a significant contribution to the scattering cross-section.

In the case of $\alpha_l < 0$ (i.e., for the value $\tilde{\alpha} < 2l+1, l \geq 1$), the situation is different. Here, according to Eq. (4), $E_R > 0$ and the left part of Eq. (3) is imaginary. The next iteration allows us to obtain the imaginary part of the amplitude's pole, $E_l = E_R - i\Gamma_R/2$, which determines the width of the quasi-stationary state considered:

$$\Gamma_R \approx \frac{2\hbar^2}{m\left|r_l\right|}k_R^{2l+1} \sim (k_R R)^{2l+1}\frac{\hbar^2}{mR^2}, \quad k_R = \frac{1}{\hbar}\sqrt{2mE_R} \tag{6}$$

The dependence of Γ_R on k_R is determined by the energy-dependence of the transmission coefficient of the centrifugal barrier:

$$\Gamma_R \propto D_l \sim \exp\left\{-2\int_R^b \sqrt{\frac{(l+1/2)^2}{r^2} - k_R^2}dr\right\} \sim$$
$$\exp\left\{-(2l+1)\ln\frac{l+1/2}{k_R R}\right\} \propto (k_R R)^{2l+1}$$

$b = (l+1/2)/k_R$ is the quasi-classical turning point. Compare to Problem 9.30.
Now the partial scattering cross-section, $\sigma_l(E)$, is large for energies in a narrow region of width $\sim \Gamma_R$ around E_R, and is

[0] [350] Since $l \geq 1$, the s-level for $\tilde{\alpha} < 1$ is virtual.

$$\sigma_l(E) \approx \frac{\pi(2l+1)}{k^2} \frac{\Gamma_R^2}{(E-E_R)^2 + \Gamma_R^2/4} \tag{7}$$

It is large, $\sigma_l \sim k_R^{-2} \gg R^2$, and is much larger than the scattering cross-section in the s-wave $\left(\sigma_0 \sim \pi R^2\right)$, so the total cross-section is $\sigma \approx \sigma_l$. Outside this energy region, for $|E - E_R| \gg \Gamma_R$, the cross-section is described analogously to Eq. (5), with the change $(E + |E_R|)^2 \to (E - E_R)^2$. Therefore, the estimate of the scattering cross-section given above for $a_l > 0$ is the same as for $a_l < 0$ considered here.

GKKG.13.47

On the basis of the specific model, including a potential well of strength U_0 and radius R that is surrounded by a δ-barrier $\bar{U}(r) = \alpha\delta(r - R)$ (Fig. 13.4), investigate how
the existence of a weakly-penetrating barrier [351] (in this model, $m\alpha R/\hbar^2 \gg 1$) affects scattering of slow particles int he s-state.

Hint: Use the effective range expansion, paying attention to the effect of the weakly penetrable barrier on the effective range of the interaction, r_0.

Solution

We use the effective range expansion and calculate the parameters of low-energy scattering, a_0 and r_0. The wavefunction $\chi_0 = rR_0(r)$ for $E = 0$ and $l = 0$ has the form:

$$\chi_0(r) = \begin{cases} C \sin \kappa_0 r, r < R, \kappa_0 = \frac{1}{\hbar}\sqrt{2mU_0} \\ 1 - \frac{r}{a_0}, \quad r > R \end{cases}$$

Matching the solution at the point $r = R$ (see Problem 2.6), we obtain:

$$C \sin \lambda = 1 - \frac{R}{a_0}, \quad \frac{R}{a_0} + \lambda C \cos \lambda = \tilde{\alpha}\left(\frac{R}{a_0} - 1\right) \tag{1}$$

where $\lambda = \kappa_0 R$ and $\tilde{\alpha} = 2m\alpha R/\hbar^2$. Hence, we find the scattering length:

$$a_0 = R\left(1 - \frac{1}{\tilde{\alpha} + \lambda \cot \lambda}\right) \tag{2}$$

When the inequality $\tilde{\alpha} \gg 1$ is fulfilled, we generally have $a_0 \approx R$, which corresponds to the scattering length of an impenetrable sphere of radius R (a physically intuitive result due to the small penetrability of the barrier).

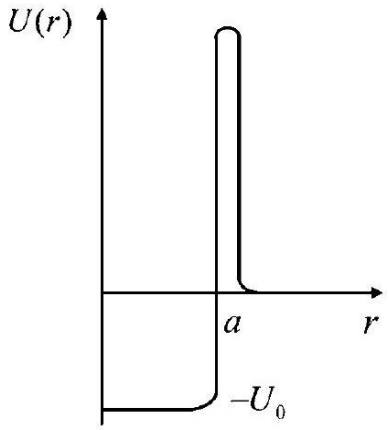


Fig. 13.4

A large difference from the scattering length of an impenetrable sphere appears if λ is close to $n\pi$, with $n = 1, 2, ...$ Writing here $\lambda = n\pi + \gamma$, where $|\gamma| \ll 1$, we obtain:

$$a_0 \approx R\left[1 - \frac{1}{\tilde{\alpha} + n\pi/\gamma}\right] \tag{3}$$

[0] [351] For physical applications, especially interesting is the case where such barrier originates from the Coulomb repulsion of charged particles. But due to the slow decrease of the Coulomb potential, this case needs special consideration.

When $\gamma \approx \gamma_{0,n} = -n\pi/\tilde{\alpha}$, the scattering length is large, $|a_0| \gg R$, and becomes infinite for $\gamma = \gamma_{0,n}$. Such potential parameters correspond to the appearance of a level with energy $E = 0$ (the nth level). In the case of $|a_0| \gg R$, slow particle scattering is resonant.

Now calculate the effective range, r_0. According to Eq. (1), for $a_0 = \infty$ we have $C \approx (-1)^{n+1}\tilde{\alpha}/n\pi$, and from the equation for effective range, r_0, at the threshold of s-level formation,

$$r_0 = 2\int_0^\infty \left(1 - \chi_0^2(r)\right) dr, \quad \chi_0 = 1 \text{ for } r \to \infty$$

(compare Problem 13.43 for the case $a_0 = \infty$), we find:

$$r_0 = R\left(2 - C^2\right) \approx -C^2 R \approx -\left(\frac{\tilde{\alpha}}{n\pi}\right)^2 R \tag{4}$$

Unlike the case of s-scattering by a well without a barrier (where $r_0 \sim R$ and $r_0 > 0$; see Problem 13.43), the effective range at the threshold is large, $|r_0| \gg R$, and negative, $r_0 < 0$. Therefore, the term containing the effective range in Eq. (XIII.15) is essential [352] for description of the resonant s-scattering. The situation is analogous to the one that takes place for scattering of particles with non-zero angular momenta, and the physical reason for this similarity is the existence of the weakly-penetrable δ-barrier that for $l = 0$ plays the same role as the centrifugal potential for $l \neq 0$.

Both the amplitude of resonant scattering,

$$f \approx f_0 = \frac{1}{-\frac{1}{a_0} + \frac{1}{2}r_0 k^2 - ik} \tag{5}$$

and the scattering cross-section, $\sigma \approx 4\pi |f_0|^2$, have a pronounced energy dependence, whose character depends on the relation among the three small parameters $kR \ll 1$, $R/|a_0| \ll 1, R/|r_0| \ll 1$. Let us consider two cases.

1. If $|a_0| \gg |r_0|$, then

$$\sigma \approx \frac{4\pi}{\left(\frac{1}{a_0}\right)^2 + k^2 + \frac{1}{4}r_0^2 k^4} \tag{6}$$

so that the scattering cross-section is almost independent of the sign of the scattering length. In the regime with $k \ll 1/|r_0|$, the term containing the effective range, as in the ordinary s-scattering, acts as a correction. It begins to play an important role for $k > 1/|r_0|$.

[352] Let us note that $|r_0| \gg R$ holds only of there exists a "shallow" level in the system.

2) In the case of $|a_0| \ll |r_0|$, scattering strongly depends on the sign of the scattering length. For $a_0 > 0$, we have (in the denominator of Eq. (5), we could neglect the $-ik$ term):

$$\sigma(E) \approx 4\pi\left(\frac{\hbar^2}{mr_0}\right)^2 \frac{1}{(E+\varepsilon)^2}, \quad \varepsilon = -\frac{\hbar^2}{ma_0 r_0} > 0 \tag{7}$$

The cross-section is also described by an analogous equation (but with $\varepsilon \equiv -E_R < 0$) if $a_0 < 0$, except for a narrow region of energies [353], $|E - E_R| \sim \Gamma_R$, where

$$\sigma(E) \approx \frac{\pi}{k_R^2} \frac{\Gamma_R^2}{(E - E_R)^2 + \Gamma_R^2/4} \tag{8}$$

$$\Gamma_R = \frac{2\hbar^2 k_R}{m|r_0|} = \frac{2(n\pi\hbar)^2 k_R}{m\tilde{\alpha}^2 R} \tag{9}$$

Parameters E_R and Γ_R determine the position and width of the quasi-discrete level; the value of the width is connected to the penetrability of the δ-barrier. Compare to the previous problem, and also with Problem 13.48.

GKKG.13.48

Find the partial amplitude of s-wave scattering in the potential $U(r) = \alpha\delta(r - R)$. In the case of a weakly-penetrable δ-barrier, determine, $E_{R,n}$, and the widths, $\Gamma_{R,n}$, of the lowest quasi-discrete s-levels (with $E_{R,n} \sim \hbar^2/mR^2$).

Compare the scattering cross-section from the δ-sphere and impenetrable sphere. What is the difference, $\Delta\sigma(E)$, between these cross-sections if the energy is close to the energy of the quasi-discrete level?

Solution

The Schrdinger equation and its s-wave solution are

$$\chi'' - \tilde{\alpha}\delta(r-R)\chi + k^2\chi = 0, \quad \tilde{\alpha} = \frac{2m\alpha}{\hbar^2},$$
$$\chi(r) = \begin{cases} A\sin kr, & r < R, \\ \left(S_0 e^{ikr} - e^{-ikr}\right), & r > R. \end{cases}$$

Matching at the point $r = R$ (see Problem 2.6), we find

$$S_0 = e^{2i\delta_0} = e^{-2ikR}\frac{\tilde{\alpha}R\sin kR + kR\cos kR + ikR\sin kR}{\tilde{\alpha}R\sin kR + kR\cos kR - ikR\sin kR} \tag{1}$$

If the conditions $\tilde{\alpha}R \gg 1$ and $kR \sim 1$ (or more precisely, $kR \ll \tilde{\alpha}R$) are fulfilled, then from Eq. (1) we generally have $S_0 \approx e^{-2ikR}$, i.e., $\delta_0 \approx -kR$, which corresponds to the scattering from an impenetrable sphere (see Problem 13.45).

The case of particle energies for which $kR \approx n\pi$ with $n = 1, 2, ...$ needs special consideration, and in Eq. (1) we cannot simply replace the fractional factor by 1. Writing $kR = n\pi + \gamma$, with $|\gamma| \ll 1$, we have

$$\tilde{\alpha}R\sin kR + kR\cos kR - ikR\sin kR \approx (-1)^n(\tilde{\alpha}R\gamma + n\pi - in\pi\gamma) \approx$$
$$(-1)^n(\tilde{\alpha}R - in\pi)\left(kR - n\pi + \lambda + i\lambda^2\right)$$

where $\lambda = n\pi/\tilde{\alpha}R \ll 1$. Equation (1) becomes

$$S_0 \approx e^{-2ikR}\frac{kR - n\pi + \lambda - i\lambda^2}{kR - n\pi + \lambda + i\lambda^2} \tag{2}$$

Multiplying both the numerator and denominator by

$$(kR + n\pi - \lambda)\frac{\hbar^2}{2mR^2} \approx \frac{n\pi\hbar^2}{mR^2}$$

we transform Eq. (2) to a more convenient form,

$$S_0 \approx e^{2i\delta_0^{(0)}}\frac{E - E_{R,n} - i\Gamma_{R,n}/2}{E - E_{R,n} + i\Gamma_{R,n}/2} \tag{3}$$

where $\delta_0^{(0)} = -kR$, and

$$E_{R,n} = \frac{\pi^2 n^2\hbar^2}{2mR^2}\left(1 - \frac{2}{\tilde{\alpha}R}\right)$$
$$\Gamma_{R,n} = \frac{2\pi^2 n^2\hbar^2}{mR^2}\frac{n\pi}{(\tilde{\alpha}R)^2} \ll E_{R,n}$$

Equation (3) has a familiar form for resonant scattering from a quasi-discrete level. $\delta_0^{(0)}$ describes the phase of potential scattering (i.e., phase far from resonance), while $E_{R,n}$ and $\Gamma_{R,n}$ give the position and the width of the quasi-discrete level. Therefore:

1. the phase of potential scattering coincides with the scattering phase for an impenetrable sphere of radius R;

2. the position, $E_{R,n}$, of the quasi-discrete levels almost coincides with the levels in an infinitely deep well of radius R;

3. the level width, which determines the lifetime of the quasi-stationary state, could be written in the form:

$$\Gamma_{R,n} = \frac{\hbar}{\tau_n} \equiv \hbar DN = \hbar \cdot 4\lambda^2 \cdot \frac{\pi n\hbar}{2mR^2}$$

where D is the transmission coefficient (for a single collision) of the δ-barrier for an energy equal to $E_{R,n}$ (see Problem 2.30), while $N = v/2R = \pi n\hbar/2mR^2$ gives the number of times the particle hits the "wall" per unit of time.

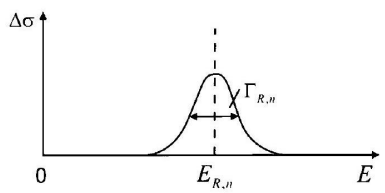


Fig. 13.5

From physical considerations, we should assume that analogous results take place for non-zero values of the angular momentum. So, for $kR \ll \tilde{\alpha}R$, the scattering cross-section on the δ-sphere almost coincides with that on the impenetrable sphere of the same radius, except for narrow regions, ΔE, in the vicinity of quasi-discrete levels. Now, the partial cross-section is described by the expression:

$$\sigma_l = 4\pi(2l+1)\frac{1}{k^2}\left|S_l - 1\right|^2$$

Note that there is no scattering with the angular momentum $l = 0$ from the impenetrable sphere for particles with energy close to the resonant energy $E_{R,n}$ of the s-level (here $\delta_0^{(0)} \approx n\pi$). Hence, we see that the difference between the scattering cross-sections of the δ - and the impenetrable sphere in the vicinity of a quasi-discrete s-level is equal to (Fig. 13.5)

$$\Delta\sigma = \pi R^2 \frac{\Gamma_{R,n}^2}{n^2\pi^2\left[\left(E - E_{R,n}\right)^2 + \Gamma_{R,n}^2/4\right]} > 0$$

GKKG.13.49

Parameters of a potential $U_0(r)$ are chosen so that there exists a zero-energy bound state with the angular momentum l in it (the scattering length is $a_l^{(0)} = \infty$). Find the scattering length, a_l, in this partial wave, for a small change of the potential by $\delta U(r)$.

Using the result obtained, discuss how the dependence of the level position on the perturbation, $\delta U(r)$, differs in the $l = 0$ case from the $l \neq 0$ case. Compare to Problems 4.27 and 4.28.

Solution

Let $\chi_l^{(0)}(r)$ and $\chi_l(r) = rR(r)$ be the zero-energy solutions to the Schrdinger equation with the potentials $U_0(r)$ and $U_0(r) + \delta U(r)$ respectively, normalized by the following conditions (compare to Problem 13.39):

$$\chi_l^{(0)} = r^{-l} \text{ and } \chi_l = r^{-l} - r^{l+1}\left\{(2l-1)!!(2l+1)!!a_l\right\}^{-1} \text{ for } r \to \infty$$

If we write the Schrdinger equation for $\chi_l^{(0)}$ and χ_l, and multiply the first equation by χ_l and the second one by $\chi_l^{(0)}$, then subtract one from the other term by term, and integrate the result over r from 0 to ∞, we find:

$$\frac{\hbar^2}{2[(2l-1)!!]^2 m a_l} = -\int_0^\infty \delta U \chi_l \chi_l^{(0)} dr \approx -\int_0^\infty \delta U \left(\chi_l^{(0)}\right)^2 dr \tag{1}$$

Compare this to the analogous transformation in Problem 13.31. We emphasize that relation (1) is valid for any value of angular momentum.

Using the result obtained and the effective range expansion (XIII.15), from the condition $\cot\delta_l\left(E_l\right) = i$ we can find the position of the pole in the partial scattering amplitude, which determines the change of the level $E_l^{(0)} = 0$ under the influence of the perturbation. If $l = 0$, we have:

$$\kappa_0 = -i\sqrt{\frac{2mE_0}{\hbar^2}} \approx \frac{1}{a_0}$$

and for a positive scattering length $a_0 > 0$ (for $\delta U < 0$), we obtain the known result:

$$E_0 \approx -\frac{2m}{\hbar^2}\left[\int_0^\infty \delta U \left(\chi_0^{(0)}(r)\right)^2 dr\right]^2 \tag{2}$$

Compare to Problem 4.27. In the case $a_0 < 0$, we also have $\kappa_0 < 0$, so that the level E_0 is virtual. We emphasize that the s-wave scattering cross-section depends weakly on the sign of $\delta U(r)$ (see Eq. (XIII.16)).

Now, consider the case with $l \neq 0$. Using Eq. (1) and the result of Problem 13.44 for the effective range of the interaction, r_l, at the threshold where a new bound state appears, we see that the level shift (determined by the poles of the partial amplitude),

$$E_l \approx -\frac{\hbar^2}{m a_l \left|r_l\right|}, \quad l \geq 1 \tag{3}$$

is linear in δU and is described by first-order perturbation theory (compare to Problem 4.28). For $a_l > 0$, the level is real with $E_l < 0$. If $a_l < 0$, then $E_l > 0$ determines the energy of a quasi-stationary state. Its width is

$$\Gamma_l \approx \frac{2\hbar^2}{m\,|r_l|}\left(\frac{2mE_l}{\hbar^2}\right)^{l+1/2} \tag{4}$$

In the case of $l \neq 0$, the nature of resonant scattering depends strongly on the sign of $\delta U(r)$. See, for example, Problem 13.46.

17.4.4 Problems about scattering of fast particles; Eikonal approximation

(углубленный метод, пару задач имеет смысл решить, набивать в них руку не целесообразно.)

GKKG.13.50 Derivation for scattering

Derive Eq. (XIII.18) for the scattering amplitude of fast particles by summing up the non-perturbative series, $f = \sum\limits_n f^{(n)}$, derived in Problem 13.10 (see Eq. (2) there).

Solution

The Fourier components of the potential, $\tilde{U}(\boldsymbol{\kappa})$ are essentially different from zero only for $\kappa R \lesssim 1$(R is the radius of the potential). So, for fast particles, $kR \gg 1$, and small scattering angles, $qR = |\mathbf{k} - \mathbf{k}_0| \lesssim 1$, the integrals over $\boldsymbol{\kappa}_k$ in this equation are dominated by the integration domains where $|\boldsymbol{\kappa}_k - \mathbf{k}_0| \lesssim 1/R$. Writing

$$\boldsymbol{\kappa}_k = \mathbf{k}_0 + \tilde{\kappa}_k^{\parallel}\mathbf{n}_0 + \boldsymbol{\kappa}_k^{\perp}$$

where $\mathbf{n}_0 = \mathbf{k}_0/k_0$ and $\boldsymbol{\kappa}_k^{\perp} \perp \mathbf{n}_0$, then for the energy denominators we have the approximate expression:

$$\kappa_k^2 - k_0^2 - i\varepsilon \approx 2k_0\tilde{\kappa}_k^{\parallel} - i\varepsilon \tag{1}$$

We neglected the terms $\left(\tilde{\kappa}_k^{\parallel}\right)^2$ and $\left(\kappa_k^{\perp}\right)^2$ in comparison to $2k_0\tilde{\kappa}_k^{\parallel}$, which leads to an error $\sim 1/kR$. Now we substitute the Fourier components of the potential into Eq. (2) from Problem 13.10:

$$\tilde{U}\left(\boldsymbol{\kappa}_k - \boldsymbol{\kappa}_{k-1}\right) = \iiint U\left(\boldsymbol{\rho}_k, z_k\right)\exp\left\{-i\left[\left(\tilde{\kappa}_k^{\parallel} - \tilde{\kappa}_{k-1}^{\parallel}\right)z + \left(\tilde{\boldsymbol{\kappa}}_k^{\perp} - \tilde{\boldsymbol{\kappa}}_{k-1}^{\perp}\right)\cdot\boldsymbol{\rho}_k\right]\right\}d^2\rho_k dz_k$$

Recall the following identity for the delta-function:

$$\iint \exp\left\{i\left(\boldsymbol{\rho}_{k+1} - \boldsymbol{\rho}_k\right)\cdot\boldsymbol{\kappa}_k^{\perp}\right\}d^2\kappa_k^{\perp} = (2\pi)^2\delta\left(\boldsymbol{\rho}_{k+1} - \boldsymbol{\rho}_k\right)$$

Now integrating over $\boldsymbol{\kappa}_k^{\perp}$, and using the δ-function to integrate over $\boldsymbol{\rho}_k$, we see that in all factors of $U\left(\boldsymbol{\rho}_k, z_k\right)$, the values $\boldsymbol{\rho}_k$ (with different k) become the same. Finally, using the integral

$$\int \frac{\exp\left\{i\left(z_{k+1} - z_k\right)\kappa_k^{\parallel}\right\}}{2k_0\kappa_k'' - i\varepsilon}d\kappa_k^{\parallel} = \frac{i\pi}{k_0}\eta\left(z_{k+1} - z_k\right)$$

($\eta(z)$ is the step function; see Problem 13.14), we find (for $k = k_0$):

$$f^{(n)} \approx \frac{k}{2\pi i}\left(-\frac{im}{\hbar^2 k}\right)^n \int\limits_{-\infty}^{z_2} dz_1 \int\limits_{-\infty}^{z_3} dz_2 \ldots \int\limits_{-\infty}^{\infty} dz_n \times$$
$$\iint U\left(\boldsymbol{\rho}, z_1\right)\ldots U\left(\boldsymbol{\rho}, z_n\right)e^{-i\mathbf{q}_\perp\cdot\boldsymbol{\rho}}d^2\rho \tag{2}$$

In the exponent we neglected the term $-iq_{\parallel}z_n$, because $q_{\parallel} \ll q_{\perp}$ (compare to Problem 13.2). In this expression we extend integration to infinite limits over all z_k if we introduce the factor $(n!)^{-1}$. As a result, we obtain the scattering amplitude in the eikonal approximation:

$$f \approx \frac{k}{2\pi i} \iint \left\{ \sum_{n=1}^{\infty} \frac{1}{n!} \left(-\frac{im}{\hbar^2 k} \right)^n \left[\int_{-\infty}^{\infty} U(\boldsymbol{\rho}, z) dz \right]^n \right\} e^{-i\mathbf{q}_\perp \cdot \boldsymbol{\rho}} d^2\rho =$$

$$= \frac{ik}{2\pi} \iint \left\{ 1 - \exp\left\{ -\frac{i}{\hbar v} \int_{-\infty}^{\infty} U(\boldsymbol{\rho}, z) dz \right\} \right\} e^{-i\mathbf{q}_\perp \cdot \boldsymbol{\rho}} d^2\rho. \tag{3}$$

In conclusion, we discuss the conditions of applicability of Eq. (3), which follow form the above derivation. Omission of the terms $q_\parallel z \leq q^2 R/k \approx k\theta^2 R \ll 1$ in the exponent of Eq. (2) implies small scattering angles $\theta \ll 1/\sqrt{kR}$. Since $kR \gg 1$, then this region includes scattering angles $\theta \lesssim 1/kR$, which dominate the total cross-section. This, as we noted in the context of Eq. (1), contributes an error $\sim 1/kR$. But the quantity of interest appears in the exponent of Eq. (3). So the condition of its applicability becomes

$$\frac{1}{\hbar v} UR \cdot \frac{1}{kR} \ll 1, \quad \text{i.e.} \quad |U(r)| \ll E.$$

GKKG.13.51

Prove that the total scattering cross-section of fast particles, $kR \gg 1$, in a potential, $U(r)$, of radius R follows from the equation:

$$\sigma(E) = 4\pi \int_0^{\infty} \left\{ 1 - \cos\left[\frac{m}{k\hbar^2} \int_{-\infty}^{\infty} U\left(\sqrt{\rho^2 + z^2} \right) dz \right] \right\} \rho d\rho \tag{1}$$

independently of the relation between particle energy and the characteristic strength of the potential, i.e., the validity of the equation in question does not require that the condition of applicability of the eikonal approximation, $E \gg |U(r)|$, is necessarily satisfied. [354]

Use this result to calculate the scattering cross-section from the potential barrier (or well) with $U = U_0$ for $r < R$ and $U = 0$ for $r > R$.

Solution

Eq. (1) can be derived by combining the optical theorem and the eikonal approximation, Eq. (XIII.18). The condition for its applicability for fast particles is the inequality
$|U(r)| \ll E$, which is valid for a large fraction of scattering angles, $\theta \lesssim 1/kR$ (see the previous problem). In the case of a "strong" potential, for which $|\widetilde{U}(r)| \gtrsim E$ when $r \sim R$, scattering into the angles $\theta \sim 1/kR$ is not described by the eikonal expression. But for forward scattering, corresponding to the angle $\theta = 0$, the amplitude,

$$f(E, \theta = 0) = \frac{1}{2ik} \sum_l (2l+1) \left(e^{2i\delta_l} - 1 \right) \tag{2}$$

still has the eikonal form (the approximation actually remains valid for the region of small scattering angles $\theta \ll 1/kR$, for as long as we can put $P_l \approx 1$ in the amplitude expansion over partial waves, Eq. $f(k,\theta) = \sum_{l=0}^{\infty} (2l+1)\varphi_l(E) P_l(\cos\theta)$; $\varphi_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k(\cot\delta_l - i)}$ and until the oscillations in the Legendre polynomials with $l \lesssim kR$ begin to play out). To see this, recall that the eikonal equation for the scattering amplitude follows from the quasi-classical expressions for the phase shifts, Eq. (XIII.14). In the case of a "strong" potential, we should use the more general expression, (XIII.13). But this fact is not reflected in the value of the forward scattering amplitude, (2). For the values of l in the sum, Eq. (2), for which $|U(r_0)| \geq E$ (r_0 is the quasi-classical turning point in Eq. (XIII.13)), the phase shifts have the following properties: they are large, $|\delta_l| \gg 1$, and change rapidly with increase in l, $|\delta_{l+1} - \delta_l| \geq 1$. These properties follow both from Eq. (XIII.13) and from [355] Eq. (XIII.14). This leads to the fact that in the corresponding part of sum (2), the contribution of the term with $\exp(2i\delta_l)$ is negligible due to fast oscillations. This happens independently of which expression is used, correct (XIII.13) or "incorrect" Eq. (XIII.14). For values of l such that $|U(r_0)| \ll E$, (XIII.14) is still valid. Therefore the amplitude of forward scattering for fast particles is still described by the eikonal expression, even if the condition $|U(r_0)| \ll E$ breaks down. The statement of the problem follows from the optical theorem. The unitary properties of the scattering amplitude in the eikonal approximation are discussed in Problem 13.76.

In the case of a potential barrier (or a well), we find:

$$\sigma(E) = 4\pi \int_0^R \left[1 - \cos\left(\xi\sqrt{1 - \frac{\rho^2}{R^2}}\right)\right] \rho d\rho =$$
$$2\pi R^2 \left[1 - \frac{2}{\xi^2}(\xi \sin\xi + \cos\xi - 1)\right] \tag{3}$$
$$\xi = \frac{2mU_0 R}{k\hbar^2}$$

This integral is calculated using the substitution $x = \sqrt{1 - \rho^2/R^2}$. For the values $\xi \ll 1$ from Eq. (2), the result of the Born approximation follows

[355] For example, according to Eq. (XIII.14) we have:

$$|\delta_{l+1} - \delta_l| \sim \left|\frac{\partial}{\partial l}\delta_l\right| \sim \frac{m}{\hbar^2 k} |U(r_0)| \frac{l}{k^2 R} \sim \frac{m|U(r_0)|}{\hbar^2 k^2}$$
$$\sigma(E) \approx \pi R^2 \left(\frac{mU_0^2 R^2}{\hbar^2 E}\right) \ll \pi R^2$$

for fast particles (see Problem 13.1), while for $\xi \gg 1$ we have $\sigma \approx 2\pi R^2$, the known result for the scattering cross-section of fast particles from an impenetrable sphere (see Problem 13.57).

GKKG.13.52

Find the total scattering cross-section in the potential $U(r) = \alpha/r^\nu$ with $\nu > 2$ and $\alpha > 0$, for energy $E \to \infty$. Compare to Problem 13.2.

Solution

Let us use the quasi-classical equation for the scattering cross-section from the previous problem. We will also use the integral:

$$\int_{-\infty}^{\infty} U\left(\sqrt{\rho^2 + z^2}\right) dz = 2\alpha\rho^{-\nu+1} \int_0^\infty \frac{du}{(1+u^2)^{\nu/2}} =$$
$$\frac{\sqrt{\pi}\alpha}{\rho^{\nu-1}} \frac{\Gamma((\nu-1)/2)}{\Gamma(\nu/2)}$$

(By the substitution $1 + u^2 = 1/t$, this integral could be transformed to the Euler integral, giving the β-function, $B(x, y)$, with $x = 1/2$ and $y = (\nu - 1)/2$.) We can perform the integration [356] over ρ and obtain

$$\sigma(E) = 2\pi\Gamma(\lambda) \sin\frac{\pi\lambda}{2} \left[\frac{\sqrt{\pi}\alpha}{\hbar v} \frac{\Gamma((\nu-1)/2)}{\Gamma(\nu/2)}\right]^\mu \propto E^{-1/(\nu-1)} \tag{1}$$

where $\lambda = (\nu - 3)/(\nu - 1)$ and $\mu = 2/(\nu - 1)$.
As is seen from Eq. (1), the decrease of the scattering cross-section for $E \to \infty$ is slower than is required for the applicability of the Born approximation, where $\sigma \propto 1/E$. This is because in the scattering of fast particles in the potential $U \propto r^{-\nu}$ with $\nu > 2$, small distances play the dominant role (small impact parameter), and the potential cannot be considered as a perturbation. For large values of energy $E \to \infty$, Eq. (1) is valid for a fairly arbitrary potential, which has the form considered only at small distances. See that for the values $\nu \to 2$, the energy dependence of the cross-section is determined by Eq. (1) and "matches" the result obtained in the Born approximation.

[356] First we make the substitution $x = \rho^2$ and perform integration by parts, which leads to the integral of the form $\int \frac{1}{x^s} \sin\left(\frac{a}{x^s}\right) dx$ with $s = (\nu - 1)/2$. Expressing the sine as a sum of two complex exponentials and making the substitution $v = \pm ia/x^s$, we obtain the integrals that give the Γ-function.

GKKG.13.53

Consider a "potential" of the form $U = g(E)e^{-r/R}$, with the interaction constant, [357] which scales as a power-law with energy, $g(E) = g_0 \left(E/E_0\right)^n$. Prove the inequality

$$\sigma(E) \leq \sigma_0 \ln^2 \left(\frac{E}{E_0}\right)$$

for the energy-dependence of the scattering cross-section in the large-energy limit, $E \to \infty$.

Solution

To calculate the scattering cross-section we use the result of Problem 13.51. The quasiclassical phase shift for large values of the impact parameter $\rho \gg R$ is equal to

$$\delta(\rho) = \frac{g(E)}{2\hbar v} \int\limits_{-\infty}^{\infty} \exp\left\{-\frac{1}{R}\sqrt{\rho^2 + z^2}\right\} dz \approx \frac{g_0}{2\hbar v}\sqrt{2\pi\rho R}\left(\frac{E}{E_0}\right)^n e^{-\rho/R} \tag{1}$$

To calculate this integral, use the expansion: $\sqrt{\rho^2 + z^2} \approx \rho + z^2/2\rho$.
Let us denote by ρ_0 the value of ρ for which the following condition for the phase shift is satisfied: $\delta\left(\rho_0\right) = 1$. In the case $n > 1/2$ and at large energies, we have $\rho_0 \gg R$ (for $E \to \infty, \rho_0 \to \infty$ as well). Now we note that the phase shift is a sharp, rapidly decreasing function of ρ. For calculation of the cross-section using the equation from Problem 13.51, we can completely neglect both the contribution of integration domain $\rho > \rho_0$ (since there, $\delta \approx 0$). On the other hand, in the other domain $\rho < \rho_0$, we can neglect the term corresponding to the fast-oscillating factor, $\cos 2\delta(\rho)$ (because, $\delta \gg 1$). As a result, we obtain $\sigma(E) = 2\pi\rho_0^2(E)$. Thus, using Eq. (1), we find that

$$\sigma(E) \approx \sigma_0 \ln^2 \left(\frac{E}{E_0}\right), \text{ where } \sigma_0 = 2\pi\left(n - \frac{1}{2}\right)^2 R^2 \tag{2}$$

for $n > 1/2$. To calculate approximately $\rho_0(E)$ from the relation $\ln \delta\left(\rho_0\right) = 0$, we neglected the term $\ln\left(\rho_0/R\right)$ in comparison to ρ_0/R. Finally, we mention that for the values $n < 1/2$, the scattering cross-section decreases with the increase of E.

GKKG.13.54

In the eikonal approximation, find the amplitude and differential scattering cross-section for the Coulomb potential, $U = \alpha/r$, in the limiting case opposite to that

[357] Let us note that the spin-orbital interaction, $\hat{U} = \hat{\mathbf{s}} \cdot \hat{\mathbf{l}} f(r)$, increases $\propto \sqrt{E}$ with E. Compare to Problem 13.59. The restriction on the increase of cross-section is known as the Froissart theorem in the theory of strong interactions in elementary particle physics.
required for the validity of the Born approximation: i.e., consider $|\alpha|/\hbar v \gg 1$. Compare to Problem 13.1.
Hint: To calculate the scattering amplitude, introduce a cut-off for the Coulomb potential at some large, but finite, distance R (i.e., put $U = 0$ for $r > R$).

Solution

According to Eq. (XIII.19), for the values $\rho \ll R$, we have

$$\delta(\rho) = -\frac{\alpha}{2\hbar v} \int\limits_{-R}^{R} \frac{dz}{\sqrt{\rho^2 + z^2}} \approx -\frac{\alpha}{\hbar v} \ln \frac{2R}{\rho} \tag{1}$$

and for the $q \neq 0$ scattering amplitude from Eq. (XIII.19), we obtain the relation:

$$f(E, q) = \frac{k}{2\pi i} \int\limits_0^{\infty} \int\limits_0^{2\pi} e^{iS(\rho,\varphi)} \rho d\rho d\varphi$$

where

$$S = \frac{2\alpha}{\hbar v} \ln \frac{\rho}{2R} - q\rho \cos\varphi \tag{2}$$

In the case $|\alpha| \gg \hbar v$, the phase in the exponential is large, and changes rapidly with a change in ρ and φ. Hence, the integral is determined mainly by the integration domains in the vicinity of the saddle points, where the phase reaches extrema as a function of the variables ρ, φ. From this saddle point condition, we find:

$$2\alpha = \hbar v \rho_0 q \cos\varphi_0, \quad q\rho_0 \sin\varphi_0 = 0$$

Thus $\rho_0 = 2|\alpha|/\hbar v q$, and $\varphi_0 = 0$ for $\alpha > 0$ or $\varphi_0 = \pi$ for $\alpha < 0$ (here $|\alpha|/\rho_0 \ll \hbar k v$, i.e., $|U| \ll E$, which allows us to use the eikonal approximation). Expanding $S(\rho, \varphi)$ in the vicinity of the extremum (ρ_0, φ_0) with quadratic accuracy, and using the value of the Poisson integral, we obtain the scattering amplitude:

$$f(E, q) \approx -i \frac{2m|\alpha|}{\hbar^2 q^2} \exp\left\{iS\left(\rho_0, \varphi_0\right)\right\} \tag{3}$$

Therefore, the differential scattering cross-section is

$$\frac{d\sigma}{d\Omega} = \left(\frac{2m\alpha}{\hbar^2 q^2}\right)^2 \approx \frac{\alpha^2}{E^2\theta^4}$$

which coincides with the Rutherford equation (for small scattering angles, $\theta \ll 1$).
Let us note in conclusion that the need to cut off the potential and the absence of a well-defined limit for $R \to \infty$ of the scattering amplitude (but not for the differential cross-section) are connected to the slow decrease of the Coulomb potential. At large
distances, the wavefunction of the Coulomb problem is not the wavefunction of a free particle. The phase of the wavefunction gets "distorted" by the factor,

$$\Delta(r) = -\frac{\alpha}{\hbar v} \ln 2kr$$

due to the cutting off the potential at the distance $r = R$. This distortion is then "inherited" by the scattering amplitude in the form of the factor $\exp\{2i\Delta(R)\}$. Factoring it out from Eq. (3), we obtain the scattering amplitude:

$$\tilde{f}(k, q) = f e^{-2i\Delta(R)} = -\frac{2m\alpha}{\hbar^2 q^2} e^{i\varphi(k,q)}$$
$$\varphi(k, q) = -\frac{2\alpha}{\hbar v} \ln \frac{q}{2k} + \frac{2\alpha}{\hbar v} \ln \frac{|\alpha|}{\hbar v} - \frac{2\alpha}{\hbar v} + \frac{\pi}{2} \frac{\alpha}{|\alpha|} \tag{4}$$

It is now independent of the cutoff radius, and coincides, as expected, with the amplitude of Coulomb scattering: [358]

$$f_{\text{Coul}} = -\frac{\alpha}{2mv^2 \sin^2(\theta/2)} \frac{\Gamma(1 + i\alpha/\hbar v)}{\Gamma(1 - i\alpha/\hbar v)} \exp\left\{-\frac{2i\alpha}{\hbar v} \ln \sin\frac{\theta}{2}\right\}$$

In the quasi-classical case, $|\alpha|/\hbar v \gg 1$ for all scattering angles, while the eikonal approximation is applicable only for angles $\theta \ll \hbar v/|\alpha|$.

GKKG.13.55

In the eikonal approximation, express the scattering amplitude in the field of two identical potentials located at a distance a from one another, i.e., in the potential $U(\mathbf{r}) = U_0(|\mathbf{r} - \mathbf{a}/2|) + U_0(|\mathbf{r} + \mathbf{a}/2|)$, in terms of the amplitude, f_0, of scattering from a single spherically-symmetric potential, $U_0(r)$. What is the connection between the total scattering cross-section in $U(\mathbf{r})$ and that in a single potential, σ_0?

Use the result obtained to calculate the total scattering cross-section for a weakly bound system of two centers (like a deuteron), when its characteristic size is much larger than the interaction radius of a single scattering center.

Solution

In the eikonal approximation, the scattering amplitude is described by the expression:

$$f\left(k, \mathbf{q}_\perp\right) = \frac{ik}{2\pi} \iint \left\{1 - \exp\left\{-\frac{im}{\hbar^2 k} \int\limits_{-\infty}^{\infty} U(\boldsymbol{\rho}, z) dz\right\}\right\} e^{-i\mathbf{q}_\perp \cdot \boldsymbol{\rho}} d^2\rho \tag{1}$$

Using the Fourier transformation, we obtain:

$$\exp\left\{-\frac{im}{\hbar^2 k}\int\limits_{-\infty}^{\infty}U(\boldsymbol{\rho},z)dz\right\}=1+\frac{i}{2\pi k}\iint f\left(k,\boldsymbol{\kappa}_\perp\right)e^{i\boldsymbol{\kappa}_\perp\cdot\boldsymbol{\rho}}d^2\kappa_\perp \tag{2}$$

Now substituting into Eq. (1) the potential

$$U(\mathbf{r})=U_1\left(\mathbf{r}-\frac{\mathbf{a}}{2}\right)+U_2\left(\mathbf{r}+\frac{\mathbf{a}}{2}\right)$$

and transforming potentials $U_{1,2}(\mathbf{r})$ according to Eq. (2), we obtain the scattering amplitude from two centers in the eikonal approximation:

$$f\left(k,\mathbf{q}_\perp\right)=f_1\left(k,\mathbf{q}_\perp\right)\exp\left\{-\frac{i}{2}\mathbf{q}_\perp\cdot\mathbf{a}_\perp\right\}+f_2\left(k,\mathbf{q}_\perp\right)\exp\left\{\frac{i}{2}\mathbf{q}_\perp\cdot\mathbf{a}_\perp\right\}+$$
$$\frac{i}{2\pi k}\int f_1\left(k,\boldsymbol{\kappa}_\perp+\frac{\mathbf{q}_\perp}{2}\right)f_2\left(k,-\boldsymbol{\kappa}_\perp+\frac{\mathbf{q}_\perp}{2}\right)\exp\left\{-i\boldsymbol{\kappa}_\perp\cdot\mathbf{a}_\perp\right\}d^2\kappa_\perp \tag{3}$$

Here, $\mathbf{a}_\perp,\boldsymbol{\kappa}_\perp$ are vectors are perpendicular to the direction of the momentum of the incident particle, $\mathbf{n}_0$; for example, $\mathbf{a}=a_\parallel\mathbf{n}_0+\mathbf{a}_\perp$.

Now, we use Eq. (3) to calculate the elastic scattering amplitude from a bound system of two centers (i.e., on some composite particle), and average the wavefunction $\psi_0(\mathbf{a})$ of the composite system, i.e., $\int d^3a\left|\psi_0(\mathbf{a})\right|^2$ (here it is assumed that the velocity of the target particle is small with respect to the velocity of the incident particle). We also emphasize that $\psi_0(\mathbf{a})$ is the wavefunction of the composite system in its center-of-mass frame (and the target as a whole remains at rest). The radius vectors of the target particles are chosen to be equal to $\pm\mathbf{a}/2$, and it is assumed that they have identical masses (as is the case for the deuteron). The integrals that appear after the averaging are expressed in terms of the form factor of the composite system, equal to

$$F(\mathbf{q})=\int\left|\psi_0(\mathbf{r})\right|^2\exp\left\{-\frac{i}{2}\mathbf{q}\cdot\mathbf{r}\right\}d^3r$$

As a result of averaging, Eq. (3) takes the form:

$$\left\langle f\left(k,\mathbf{q}_\perp\right)\right\rangle=f_1\left(k,\mathbf{q}_\perp\right)F\left(\mathbf{q}_\perp\right)+f_2\left(k,\mathbf{q}_\perp\right)F\left(-\mathbf{q}_\perp\right)+$$
$$\frac{i}{2\pi k}\int f_1\left(k,\boldsymbol{\kappa}_\perp+\frac{\mathbf{q}_\perp}{2}\right)f_2\left(k,-\boldsymbol{\kappa}_\perp+\frac{\mathbf{q}_\perp}{2}\right)F\left(2\boldsymbol{\kappa}_\perp\right)d^2\kappa_\perp \tag{4}$$

Using the optical theorem (XIII.11), the total scattering cross-section can be expressed in terms of the forward scattering amplitude for angle $\theta=0$ (i.e., $\mathbf{q}_\perp=\mathbf{0}$), so that

$$\sigma_{tot}=\sigma_1+\sigma_2+\frac{2}{k^2}\,\mathrm{Re}\int F\left(2\boldsymbol{\kappa}_\perp\right)f_1\left(k,\boldsymbol{\kappa}_\perp\right)f_2\left(k,-\boldsymbol{\kappa}_\perp\right)d^2\kappa_\perp \tag{5}$$

where $\sigma_{1,2}$ are the scattering cross-sections of free particles hitting the target. (We should emphasize that the total scattering cross-section may also include processes, where the initial composite system breaks up).

Notice that the properties of scattering from a weakly-bound system are determined by the fact that the typical momentum, where the form factor begins to noticeably decrease, is of the order of

$$q\sim\frac{1}{R}\sim\left(\frac{\mu\varepsilon_{\mathrm{bind}}}{\hbar^2}\right)^{1/2} \tag{6}$$

where R is the size of a system, $\varepsilon_{\mathrm{bind}}$ and μ are the binding energy and reduced mass of target particles, and R is assumed to be much larger than the interaction radius. Since the characteristic values of q for scattering are of the order of the inverse interaction radius, i.e., are large in comparison to (6), then in Eq. (5) the amplitudes, $f_{1,2}$, can be factored outside of the integral at the point $\boldsymbol{\kappa}_\perp=\mathbf{0}$. Next, we perform the following transformation:

$$\int F\left(2\boldsymbol{\kappa}_\perp\right)d^2\kappa_\perp=\iiint\exp\left\{-i\boldsymbol{\kappa}_\perp\cdot\boldsymbol{\rho}\right\}\left|\psi_0(\boldsymbol{\rho},z)\right|^2d^2\rho dz d^2\kappa_\perp=$$
$$=(2\pi)^2\int\limits_{-\infty}^{\infty}\left|\psi_0(\mathbf{0},z)\right|^2dz=2\pi\int\limits_0^\infty\frac{1}{r^2}\left|\psi_0(r)\right|^2 4\pi r^2dr\equiv 2\pi\left\langle\frac{1}{R^2}\right\rangle$$

We have assumed that the angular momentum of the composite system is equal to zero, so that the wavefunctiom $\psi_0(r)$ is spherically symmetric. $\left\langle R^{-2}\right\rangle$ is the mean value of the inverse distance between the target particles squared. We obtain:

$$\sigma_{tot}=\sigma_1+\sigma_2+\Delta,\quad \Delta=\frac{4\pi}{k^2}\left\langle\frac{1}{R^2}\right\rangle\mathrm{Re}\left(f_1(k,0)f_2(k,0)\right) \tag{7}$$

In particular, if $f_{1,2}(k,0)$ are purely imaginary quantities, then, using the optical theorem for the single center amplitudes, we find:

$$\Delta = -\frac{1}{4\pi}\sigma_1\sigma_2 \left\langle \frac{1}{R^2} \right\rangle \tag{8}$$

Let us note that such a case of imaginary amplitudes corresponds to scattering from impenetrable (or "black") spheres (compare to Problems 13.57 and 13.90). Also, note that the fact that the scattering cross-section from two centers is a little smaller (since $\Delta < 0$) than $\sigma_1 + \sigma_2$, can be thought of as an effect of mutual shading one sphere by the other.

GKKG.13.56

Extend the eikonal approximation to the case of an exchange interaction, $\hat{U}_{\text{ex}}\,\psi(\mathbf{r}) \equiv U(r)\psi(-\mathbf{r})$. What is the connection between the differential and total scattering cross-
sections for the exchange potential and the corresponding ordinary potential? Compare to scattering in the Born approximation, as considered in Problem 13.3.

Solution

We will generalize the derivation of the scattering amplitude in the eikonal approximation based on the quasi-classical expression, Eq. (XIII.14), for the phase shift. If we replace the summation over partial waves by integration over the impact parameters and note that in approximation (XIII.14) for the exchange potential, the phase shift is

$$\delta_{l,ex} = (-1)^l \delta_{l,com} \tag{1}$$

then it is easy to obtain the following results.
In the region of small scattering angles, $\theta \ll 1$, the scattering amplitude for the exchange interaction is described by an equation analogous to (XIII.18), but with $\cos 2\delta_l$ instead of $e^{2i\delta_l}$; i.e.,

$$f_{ex}(k,\theta) \approx \frac{k}{\theta}\iint [\cos 2\delta(\rho) - 1]\exp\{-iq\rho\}d^2\rho = \\ -ik\int_0^\infty [\cos 2\delta(\rho) - 1]J_0(k\rho\theta)\rho d\rho \tag{2}$$

with the same function, $\delta(\rho)$.
Note that the appearance of the factor $(-1)^l$ in Eq. (1) does not change the even-in- δ_l part of the scattering amplitude. For odd functions, $\propto \sin 2\delta_{l,ex}$, a strong mutual compensation of the neighboring terms in the sum over l appears, and this part of the amplitude is negligibly small.

Let us note that amplitude (2) is imaginary and coincides with the imaginary part of the scattering amplitude for the ordinary potential $U(r)$. If we take into account the optical theorem, then their total scattering cross-sections also coincide (the same for partial scattering cross-sections σ_l).

In the case of the exchange potential, the scattering amplitude has a sharp maximum in the region of angles close to π (for scattering backwards, compare to Problem 13.3). Taking into account the relation for the Legendre polynomials $P_1(z) = (-1)^l P_l(-z)$, we find:

$$f_{ex}(k,\theta) \underset{\pi-\theta}{\approx}\underset{1}{\approx} \frac{k}{2\pi}\iint \sin 2\delta(\rho)\exp\{-i\boldsymbol{\Delta}\cdot\boldsymbol{\rho}\}d^2\rho = \\ k\int_0^\infty \sin 2\delta(\rho)J_0(k\rho(\pi-\theta))\rho d\rho \tag{3}$$

where $\boldsymbol{\Delta} = \mathbf{k} + \mathbf{k}_0$. In this region of angles, the amplitude is a real function, and coincides with the real part of the scattering amplitude from the corresponding regular
potential, with the scattering angle $\theta' = \pi - \theta \ll 1$. From Eqs. (2) and (3), we recover the same fact that the total scattering cross-sections are the same for the exchange an the corresponding ordinary potential.

GKKG.13.57

Calculate the scattering amplitude and the differential and total cross-sections for small-angle scattering ($kR\theta \lesssim 1$) of fast particles ($kR \gg 1$) on a hard sphere with radius, R. Use the quasi-classical expression (XIII.13) for the phase shift.

Solution

To calculate the scattering amplitude of fast particles, we use its expansion over partial waves, Eq. $f(k,\theta) = \sum_{l=0}^{\infty}(2l+1)\varphi_l(E)P_l(\cos\theta)$; $\varphi_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k(\cot\delta_l - i)}$, and the quasi-classical expression (XIII.13) for phase shifts. Since $U = 0$ for $r > R$, then integration by parts in Eq. (XIII.13) gives:

$$\delta_l = \left(l+\frac{1}{2}\right)\arccos\frac{l+1/2}{kR} - \sqrt{k^2R^2 - \left(l+\frac{1}{2}\right)^2}, \quad l \le L \tag{1}$$

where $L = kR - 1/2$ (here $r_0 = R$), while for the values $l > L$ we obtain (here $r_0 = (1+1/2)/k$) :

$$\delta_l = 0, \quad l > L \tag{2}$$

For $l > L$, the exact phase shift is exponentially small. This is beyond quasi-classical approximation, which yields $\delta_l = 0$. Let us also mention that, strictly speaking, we should put an additional term, $-\pi/4$, in Eq. (1). It has the same origin as the modification of the quantization rule considered in Problem 9.2 (for $l < L$ in our problem, the quasi-classical approximation is reliable up to the turning point). Let us also mention that the results obtained for δ_l need correction for values of l that are close to L, since in the vicinity of the point $r = R$, the quasi-classical approximation is not applicable, and the matching conditions require a modification. However, these conditions are not important for further calculations.

Using relations (1) and (2), it is convenient to write the scattering amplitude in the form:

$$f = f_{dif} + f_{cl}$$

where

$$f_{dif} = \frac{i}{2k}\sum_{l=0}^{L}(2l+1)P_l(\cos\theta), \quad f_{cl} = \frac{1}{2ik}\sum_{l=0}^{L}(2l+1)e^{2i\delta_l}P_l(\cos\theta)$$

This partitions the amplitude into "diffractive" and "classical" parts. We will note a few important points about this partition, since it will be important for this and the following few problems. For small scattering angles (i.e., for $\theta \ll (kR)^{-1/3} \ll 1$), we have $|f_{dif}| \gg |f_{cl}|$. The contribution of this region into the total cross-section
is πR^2. Such small-angle scattering is often referred to as diffractive, because it is similar to the diffraction of a plane-parallel light beam falling onto a non-transparent (reflecting or absorptive) screen, Fraunhofer diffraction (see also Problem 13.90). For scattering angles $\theta \gg (kR)^{-1/3}$, the diffractive amplitude f_{dif} is negligibly small. f_{cl} describes the isotropic distribution of scattered particles, $d\sigma/d\Omega \approx |f_{cl}|^2 \approx R^2/4$, so that the scattering cross-section into such angles is also πR^2 (as in classical mechanics). In the region of angles $\theta \sim (kR)^{-1/3}$, the amplitudes f_{dif} and f_{cl} are of the same order. However, the contribution of these angles to scattering is negligibly small in comparison to πR^2. Therefore, the total scattering cross-section is equal to $2\pi R^2$.

For sufficiently small scattering angles, the diffraction part of the scattering amplitude becomes dominant, and $f \approx f_{\text{dif}}$. Indeed, since the phase shifts, (1), are large, $|\delta_l| \gg 1$, and change rapidly, then in the sum for f_{cl}, a mutual compensation appears due to the oscillations of $e^{2i\delta_l}$ in different terms. Using the relation $P_l(\cos\theta) \approx J_0((l+1/2)\theta)$ for $l \gg 1, \theta \ll 1$, and replacing the summation in f_{dif} by an integration over l, we obtain ($L \approx kR$):

$$f_{dif} \approx \frac{i}{2k}\int_0^L (2l+1)J_0\left(\left(l+\frac{1}{2}\right)\theta\right)dl \approx iR\frac{J_1(kR\theta)}{\theta} \tag{4}$$

We have used the equation $\int xJ_0(x)dx = xJ_1(x)$.
Note that the diffractive part of the scattering amplitude is purely imaginary. Using the optical theorem and the relation $J_1 \approx x/2$ for $x \to 0$, we again find that the total scattering cross-section is $\sigma = 2\pi R^2$, which is two times larger than the classical cross-section (compare to Problem 13.51).

In the region of small scattering angles, the differential cross-section, $d\sigma/d\Omega = |f_{dif}|^2$, is an oscillating function of θ, and the distance between the neighboring maxima is of the order of $\Delta\theta \sim 1/kR$. Using known asymptotes of the Bessel functions, according to Eq. (4) we find:

$$\frac{d\sigma_{dif}}{d\Omega} \underset{\theta \ll 1/kR^{\frac{1}{4}}(kR)^2R^2}{\approx} \frac{d\sigma_{dif}}{d\Omega} \underset{1/kR \ll \theta \ll 1}{\approx} \frac{2R\sin^2(kR\theta - \pi/4)}{\pi k\theta^3}$$

The differential scattering cross-section has a maximum in the region $\theta \lesssim 1/kR$, and decreases fast with the increase in θ.

The total cross-section of diffraction scattering is

$$\sigma_{dif} = \int |f_{dif}|^2 \, d\Omega \approx 2\pi R^2 \int\limits_0^\infty \frac{J_1^2(kR\theta)}{\theta} d\theta = \pi R^2$$

i.e., half of the total scattering cross-section.

GKKG.13.58

The same as in the previous problem, but for not necessarily small scattering angles $\theta \gg (kR)^{-1/3}$. Compare to the result of classical mechanics.

Solution

Let us consider the classical part of the scattering amplitude,

$$f_{cl} = \frac{1}{2ik} \sum_{l=0}^{L} (2l+1) e^{2i\delta_l} P_l(\cos\theta), \quad L = kR \tag{1}$$

where δ_l is given by Eq. (1) of the previous problem.
We use a general method of calculating sums such as in Eq. (1) (which involves replacing the sum over l with an integral and using the saddle-point approximation as discussed in great detail in, e.g., the relevant chapter of the Landau and Lifshtiz theoretical physics course) and first write down the equation

$$2 \arccos \frac{l+1/2}{kR} \pm \theta = 0$$

that determines the extremum point l_0 as follows

$$l_0 + \frac{1}{2} = kR \cos\frac{\theta}{2}, \quad \delta_{l_0} = \frac{1}{2}\left(l_0 + \frac{1}{2}\right)\theta - kR \sin\frac{\theta}{2}$$

The final expression [359] for f_{cl} takes the form:

$$f_{cl} = -\frac{i}{2} R \exp\left\{-2ikR \sin\frac{\theta}{2}\right\} \tag{2}$$

Therefore,

$$\frac{d\sigma_{cl}}{d\Omega} = |f_{cl}|^2 = \frac{R^2}{4}, \quad \sigma_{cl} = \pi R^2 \tag{3}$$

which coincides with the result of classical mechanics.
In conclusion, let us refer to Fig. 13.6 for an illustration of a qualitative dependence of the scattering cross-section, $d\sigma/d\Omega$, on the angle θ for scattering of fast particles, $kR \gg 1$ (or, more precisely, for $(kR)^{1/3} \gg 1$), from an impenetrable sphere according to the results of this and the previous problems.

[359] This corresponds to a repulsive potential. The phase factor $e^{-i\pi/4}$, which appears at the transition from the summation over l to an integration, is omitted here (which, however, is not reflected in the value of the differential scattering cross-section.)

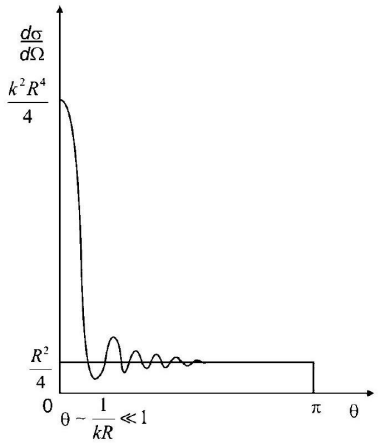


Fig. 13.6

17.4.5 Problems about scattering of particles with spin

(это усложнение, тоже это выходит за рамки минимальной подготовки и если отдельно нет исследования в этом, не вижу смысла заранее разбирать)

GKKG.13.59

The operator describing interaction of a spin-1/2 particle with an external field has the form:

$$\hat{U} = U_0(r) + U_1(r)\hat{\sigma} \cdot \hat{\mathbf{l}}$$

What is the energy dependence of the total scattering cross-section for fast particles in the Born approximation? Compare to the scattering of spinless particles.

Find the spin-dependent part of the electron scattering amplitude in the Coulomb field of a nucleus, $U_0 = -Ze^2/r$, taking into account the spin-orbital interaction, $U_1 = \left(\hbar^2/4m^2c^2r\right)\partial U_0/\partial r$

By the way, a classical analog of the spin-orbital interaction $U(r)\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{l}}$ is considered in Problem 13.60. If for a particle with spin $s = 1/2$, we write the magnetic moment in the form $\mu_0 = e\hbar/2mc + \mu'$, where e, m are the charge and mass of a particle and μ' is the anomalous magnetic moment, then the correct quantum-mechanical generalization of the classical result from Problem 13.60 is obtained by substituting the operator $\mu_0'\hat{\sigma}$ with $\mu_0' = e\hbar/4mc + \mu'$ instead of μ. See Problem 15.32.

Solution

Eqs. (XIII.1-XIII.5) are easily generalized to describe scattering of "spinfull" particles. A substitution of the interaction operator $\hat{U}$ (instead of the potential U) and unperturbed wavefunction $\psi^+_{\mathbf{k}_0} = e^{i\mathbf{k}_0\cdot\mathbf{r}}\chi_l$ (χ_l is the spin function of the particle before collision) into Eq. (XIII.5) determines a spinor amplitude of the scattered wave, $F = \hat{f}\chi$, in the Born approximation. Therefore,

$$\begin{aligned}\hat{f}(\mathbf{k}, \mathbf{k}_0) &= -\frac{m}{2\pi\hbar^2}\int e^{-i\mathbf{k}\cdot\mathbf{r}}\left[U_0(r) + U_1(r)\hat{\mathbf{l}}\cdot\hat{\boldsymbol{\sigma}}\right]e^{i\mathbf{k}_0\cdot\mathbf{r}}dV = \\ &= -\frac{m}{2\pi\hbar^2}\left\{\tilde{U}_0(q) - i\left([\mathbf{k}_0 \times \mathbf{k}]\cdot\hat{\boldsymbol{\sigma}}\right)\cdot\frac{1}{q}\frac{\partial}{\partial q}\tilde{U}_1(q)\right\} \qquad (1)\end{aligned}$$

where $\tilde{U}_{0,1}(q) = \int U_{0,1}(r)\exp\{-i\mathbf{q}\cdot\mathbf{r}\}dV$. According to Eqs. (1) and (XIII.23), the total scattering cross-section in the Born approximation is described by the expression (compare to Problem 13.1)

$$\sigma = \frac{m^2}{4\pi\hbar^4k^2}\int\limits_0^{4k^2}\left\{\left|\tilde{U}_0(q)\right|^2 + \left(k^2 - \frac{q^2}{4}\right)\left|\frac{\partial\tilde{U}_1(q)}{\partial q}\right|^2\right\}dq^2 \qquad (2)$$

Let us note that in general, the term in the differential cross-section $\propto \boldsymbol{\nu}\cdot\mathbf{P}_0$ which describes azimuthal asymmetry in scattering (see Eq. (XII.23)) disappears from the calculation of the total scattering cross-section; the cross-section, averaging over the over spin projections, does not depend on the polarization, $\mathbf{P}_0$, of the initial state. So, for fast particles we obtain: [361]

$$\sigma(E) \approx \frac{C_0}{E} + C_1 \qquad (3)$$

where

$$C_0 = \frac{m}{8\pi\hbar^2}\int\limits_0^\infty\left|\tilde{U}_0(q)\right|^2dq^2, \quad C_1 = \frac{m^2}{4\pi\hbar^4}\int\limits_0^\infty\left|\frac{\partial\tilde{U}_1(q)}{\partial q}\right|^2dq^2$$

The terms here correspond to different interactions. For a large but finite energy, they could be of the same order. But in practice, the relativistic origin of the spin-orbit interaction for electrons, yields that the second (non-decreasing with energy) term is less important in the non-relativistic case.

For electron scattering in the Coulomb field, we obtain:

$$\hat{f} = \frac{2mZe^2}{\hbar^2q^2}\left\{1 - i\frac{\hbar^2k^2}{4m^2c^2}\sin\theta(\boldsymbol{\nu}\cdot\hat{\boldsymbol{\sigma}})\right\} \qquad (4)$$

where $\boldsymbol{\nu} = [\mathbf{k}_0 \times \mathbf{k}] / |[\mathbf{k}_0 \times \mathbf{k}]|$. Note that the spin-dependent part of the scattering amplitude is small, $\sim \theta v^2/c^2$.

We now calculate the spin-dependent amplitude in the presence of spin-orbit interaction, $U_1(r) = \frac{\gamma}{r}\frac{\partial}{\partial r}U_0(r)$. Taking into account Eq. (1), let us perform the following transformations

$$\int e^{-i\mathbf{k}\cdot\mathbf{r}} U_1 \hat{\mathbf{l}} e^{i\mathbf{k}_0\cdot\mathbf{r}} dV = \int U_1 \left[\mathbf{r} \times \mathbf{k}_0\right] e^{-i\mathbf{q}\cdot\mathbf{r}} dV = -\gamma \int e^{-i\mathbf{q}\cdot\mathbf{r}} \left[\mathbf{k}_0 \times U_0(r)\right] dV =$$
$$= -i\gamma \left[\mathbf{k}_0 \times \mathbf{q}\right] \tilde{U}_0(q)$$

So, for the considered spin-orbital interaction, the scattering amplitude in the Born approximation is described by the expression:

$$\hat{f} = -\frac{m}{2\pi\hbar^2}\tilde{U}_0(q)\left(1 - i\gamma\left[\mathbf{k}_0 \times \mathbf{k}\right]\cdot\hat{\boldsymbol{\sigma}}\right) \tag{5}$$

Thereafter, using the expression $\tilde{U}_0 = -4\pi Ze^2/q^2$ for the Fourier component of the Coulomb potential and the parameter $\gamma = \hbar^2/4m^2c^2$, we obtain Eq. (4).

GKKG.13.60

Find the Born scattering amplitude and differential cross-section of fast neutrons from the Coulomb field.

Solution

Let us first find the form of the interaction between a moving magnetic dipole and an electric field in classical electrodynamics. In the initial coordinate system, there is only an electric field $\mathcal{E} = -\boldsymbol{\nabla}\phi$ with $\varphi = Ze/r$. To find its interaction with a neutron, moving with the velocity $\mathbf{v} = \mathbf{p}/M$, we pass to the frame of reference moving with the neutron. In this system, a magnetic field $\mathcal{H} \approx [\mathcal{E} \times \mathbf{v}]/c$ appears, and the interaction energy becomes becomes equal to (with $\boldsymbol{\mu}$ being the neutron magnetic moment):

$$U = -\boldsymbol{\mu}\cdot\mathcal{H} = \frac{1}{Mcr}\frac{\partial\varphi}{\partial r}\boldsymbol{\mu}\cdot\mathbf{L}, \quad \mathbf{L} = [\mathbf{r}\times\mathbf{p}] \tag{1}$$

A quantum mechanical generalization of this equation is obtained by substitutions: of $\boldsymbol{\mu}$ by spin magnetic moment operator [362] $\hat{\boldsymbol{\mu}} = \mu_0\hat{\boldsymbol{\sigma}}$, where $\mu_0 = \beta e\hbar/2Mc$ (for the neutron, the experimental value is $\beta = -1.91$), and $\mathbf{L}$ by $\hbar\hat{\mathbf{l}}$. This generalization determines the interaction operator:

$$\hat{U} = \frac{\gamma}{r}\frac{\partial\varphi}{\partial r}\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{l}}, \quad \gamma = \frac{\beta e\hbar^2}{2M^2c^2} \tag{2}$$

Using the equations for scattering amplitude with the spin-orbit interaction in the Born approximation, obtained in the previous problem, we find:

$$\hat{f} = i\frac{2Ze^2M\gamma}{\hbar^2q^2}\hat{\boldsymbol{\sigma}}\cdot[\mathbf{k}_0\times\mathbf{q}] = i\frac{\beta Ze^2}{2Mc^2}\cot\frac{\theta}{2}(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\nu}) \tag{3}$$

where $\boldsymbol{\nu} = [\mathbf{k}_0 \times \mathbf{k}] / |[\mathbf{k}_0 \times \mathbf{k}]|$ is the unit vector normal to the scattering plane. The differential cross-section, summed over the neutron's spin states, is
$$

$$\frac{d\sigma}{d\Omega} = F^*F = \chi_i^*\hat{f}^+\hat{f}\chi_i = \left(\frac{\beta Ze^2}{2Mc^2}\right)^2\cot^2\frac{\theta}{2} \tag{4}$$

$$

Here, $F = \hat{f}\chi_i$ is the spinor amplitude of the scattered wave. For a small-angle scattering, $\theta \to 0$, we have $d\sigma/d\Omega \propto \theta^{-2}$, so that the total scattering cross-section becomes infinite (this divergence of the cross-section disappears if we take into account screening of the nuclear charge).

[0][361] Note that the applicability conditions of the Born approximation for the spin-orbital interaction involve a restriction on the power law decay of $U_1(r)$ at large distances, which ensures the finiteness of the total scattering cross-section. Let us emphasize that the independence of scattering cross-section from energy for $E \to \infty$ reflects its effective increase with the increase in E, since $l_{\text{eff}} \sim kR \propto \sqrt{E}$.

[0][362] See the footnote of Problem 13.59.

GKKG.13.61

What constraints does the hermiticity property of the Hamiltonian impose on the spin-orbit interaction, $\hat{U} = U_0(r) + U_1(r)\hat{\mathbf{l}} \cdot \hat{\boldsymbol{\sigma}}$, of a spin-1/2 particle with an external field.
(1) Find in the first Born approximation polarization of particles scattered by such a potential, assuming that they were unpolarized initially. (2) Show also that if the particles were, on the contrary, polarized before the collision, the latter can result only in a rotation of the polarization vector.

Solution

The hermiticity of $\hat{U} = U_0(r) + U_1(r)\hat{\mathbf{l}} \cdot \hat{\boldsymbol{\sigma}}$ demands that the functions $U_{0,1}(r)$ are real. Their Fourier components, $\tilde{U}_{0,1}(q)$ are also real, and so are the invariant functions A and B in the expression below for the Born scattering amplitude

$$\hat{f} = A(k,\theta) + iB(k,\theta)\boldsymbol{\nu} \cdot \hat{\boldsymbol{\sigma}} \tag{1}$$

(see Eqs. (1) and (5) from Problem 13.59). So, according to the general equation (XIII.24), we find that the scattered particles remain unpolarized, $\mathbf{P} = \mathbf{0}$, if they were unpolarized initially, $\mathbf{P}_0 = \mathbf{0}$.

For the scattering of polarized particles, the final polarization vector is equal to [363]

$$\mathbf{P} = \frac{\left(|A|^2 - |B|^2\right)\mathbf{P}_0 + 2|B|^2\boldsymbol{\nu}\left(\boldsymbol{\nu}\cdot\mathbf{P}_0\right) - 2\,\mathrm{Re}\,AB^*\left[\boldsymbol{\nu}\times\mathbf{P}_0\right] + 2\,\mathrm{Im}\,AB^*\cdot\boldsymbol{\nu}}{|A|^2 + |B|^2 + 2\,\mathrm{Im}\,AB^*\nu P_0}$$

Since A and B are real functions, then

$$\mathbf{P}_B = \frac{1}{A^2+B^2}\left\{\left(A^2 - B^2\right)\mathbf{P}_0 + 2B^2\boldsymbol{\nu}\left(\boldsymbol{\nu}\cdot\mathbf{P}_0\right) - 2AB\left[\boldsymbol{\nu}\times\mathbf{P}_0\right]\right\}$$

and $\mathbf{P}_B^2 = \mathbf{P}_0^2$. This corresponds to a rotation of the polarization vector around the normal to the scattering plane; here, $\boldsymbol{\nu}\cdot\mathbf{P}_B = \boldsymbol{\nu}\cdot\mathbf{P}_0$.

[363] Note that in Eq. (1), we have adopted a convention, which includes the imaginary constant, i, in front of the coefficient, B (different conventions can be found in the literature).

GKKG.13.62

Find the polarization that appears as a result of scattering of fast $\left(Ze^2/\hbar v \ll 1\right)$ (initially unpolarized) electrons in the Coulomb field of a nucleus. Find also the induced polarization for the Coulomb scattering of initially unpolarized positrons.
Hint: Spin-orbital interaction was discussed in Problem 13.59. To calculate the amplitude in second-order perturbation theory, first consider a screened Coulomb potential, $U_0(r) = -\left(Ze^2/r\right)e^{-r/R}$, and take the $R \to \infty$ in the end of the calculation (compare to Problem 13.54).

Solution

To the first order in interaction

$$\hat{U} = U_0(r) + \frac{\hbar^2}{4m^2c^2r}\frac{\partial U_0(r)}{\partial r}\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{l}}, \quad \text{where} \quad U_0(r) = -\frac{Ze^2}{r}e^{-r/R}$$

the scattering amplitude has the form:

$$f^{(1)}(\mathbf{k},\mathbf{k}_0) = \frac{2mZe^2}{\hbar^2\left[\left(\mathbf{k}-\mathbf{k}_0\right)^2 + R^{-2}\right]}\left\{1 - i\frac{\hbar^2}{4m^2c^2}\left[\mathbf{k}_0\times\mathbf{k}\right]\cdot\hat{\boldsymbol{\sigma}}\right\} \equiv$$
$$A^{(1)} + iB^{(1)}\boldsymbol{\nu}\cdot\hat{\boldsymbol{\sigma}}. \tag{1}$$

See Eqs. (4) and (5) from Problem 13.59. Functions $A^{(1)}$ and $B^{(1)}$ are real, and so in the first order of perturbation theory there is no polarization from scattering (see Eq. (XIII.24)).
The general expression for the second-order amplitude, as in the case of spinless particles (see Problem 13.10), is

$$\hat{f}^{(2)}(\mathbf{k},\mathbf{k}_0) = \frac{1}{2\pi^2}\int \hat{f}^{(1)}(\mathbf{k},\boldsymbol{\kappa})\hat{f}^{(1)}(\boldsymbol{\kappa},\mathbf{k}_0)\frac{d^3\kappa}{\kappa^2 - k^2 - i\varepsilon} \tag{2}$$

To calculate a spin-dependent part of the scattering amplitude, $A^{(2)}$, it suffices to retain only the first-order terms in Eq. (2) (including $A^{(2)}$ into both amplitudes $f^{(1)}$ in (2) would result in the additional small relativistic factor $\sim (v/c)^2$, which is beyond the accuracy of the approximation used). Thus $A^{(2)}$ coincides with the scattering amplitude in second-order perturbation theory for the potential, $U_0(r)$. For a Yukawa potential (corresponding to the screened Coulomb interaction), it was calculated in Problem 13.12. Using Eq. (5) of this problem, we obtain (with substitution $\alpha \to -Ze^2$):

$$\operatorname{Im} A^{(2)} = \frac{4\left(Ze^2 m\right)^2}{\hbar^4 k q^2} \ln qR, \quad R \gg \frac{1}{k} \tag{3}$$

For the spin-dependent part of the amplitude, $f^{(2)}$, according to Eqs. (2) and (1) we find:

$$\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{\nu} \operatorname{Im} B^{(2)} = \frac{1}{4\pi} \left(\frac{Ze^2}{\hbar c}\right)^2 \mathbf{k} \cdot \hat{\boldsymbol{\sigma}} \int \frac{[\mathbf{q} \times \boldsymbol{\kappa}] d\Omega_\kappa}{\left[(\mathbf{k}_0 - \boldsymbol{\kappa})^2 + R^{-2}\right] [(\mathbf{k} - \boldsymbol{\kappa})^2 + R^{-2}]} \tag{4}$$

Here, we should put $|\boldsymbol{\kappa}| = |\mathbf{k}| = |\mathbf{k}_0|$ for the calculation of the imaginary part (see, for example, Problem 13.11). The corresponding integral has the form:

$$\int \frac{\boldsymbol{\kappa} d\Omega_\kappa}{\left[(\mathbf{k}_0 - \boldsymbol{\kappa})^2 + R^{-2}\right] [((\mathbf{k} - \boldsymbol{\kappa})^2 + R^{-2}]} = C_1 (\mathbf{k} + \mathbf{k}_0) + C_2 \mathbf{q} \tag{5}$$

After multiplying it by $(\mathbf{k} + \mathbf{k}_0)$, we obtain

$$(\mathbf{k}_0 + \mathbf{k})^2 C_1 = \frac{1}{2} \int d\Omega_\kappa \left\{ -\frac{1}{(\mathbf{k}_0 - \boldsymbol{\kappa})^2 + R^{-2}} - \frac{1}{(\mathbf{k} - \boldsymbol{\kappa})^2 + R^{-2}} + \frac{4k^2 + 2R^{-2}}{\left[(\mathbf{k}_0 - \boldsymbol{\kappa})^2 + R^{-2}\right] [(\mathbf{k} - \boldsymbol{\kappa})^2 + R^{-2}]} \right\}$$

The first two integrals are easily calculated, and the third one could be expressed in terms of the imaginary part of the scattering amplitude for the Yukawa potential (see Problem 13.12). As a result, we obtain for $kR \gg 1$ (remember that $|\boldsymbol{\kappa}| = k$):

$$(\mathbf{k}_0 + \mathbf{k})^2 C_1 = 2\pi \left[-\frac{1}{k^2} \ln 2kR + \frac{4}{q^2} \ln qR \right]$$

Taking into account the fact that $C_2 q$ in Eq. (5) does not contribute to integral (4), and that $(\mathbf{k}_0 + \mathbf{k})^2 = 4k^2 \cos^2(\theta/2)$, we find:

$$\operatorname{Im} B^{(2)} = \frac{1}{4} \left(\frac{Ze^2}{\hbar c}\right)^2 \frac{\sin\theta}{\cos^2(\theta/2)} \left[\frac{\ln 2kR}{k} - \frac{4k \ln qR}{q^2} \right] \tag{6}$$

Now, using Eqs. (1), (3), and (6) along with Eq. (XIII.24), we obtain the electron polarization for scattering in the Coulomb field of the nucleus:

$$\mathbf{P} \approx \frac{2}{\left(A^{(1)}\right)^2} \left\{ \operatorname{Im} A^{(2)} B^{(1)} - A^{(1)} \operatorname{Im} B^{(2)} \right\} \boldsymbol{\nu} =$$
$$2 \frac{Ze^2}{\hbar c} \frac{v}{c} \frac{\sin^3(\theta/2)}{\cos(\theta/2)} \ln\left(\sin\frac{\theta}{2}\right) \boldsymbol{\nu}; \quad \boldsymbol{\nu} = \frac{[\mathbf{k}_0 \times \mathbf{k}]}{|[\mathbf{k}_0 \times \mathbf{k}]|} \tag{7}$$

We emphasize that the cut-off, introduced for regularization purposes, disappears from the final result.

For the scattering of positrons, the polarization vector has the opposite direction (the amplitude $f^{(1)}$ changes sign, while $f^{(2)}$ remains unchanged).

GKKG.13.63

The interaction of particles with spin $s = 1/2$ in an external field has the form $\hat{U} = U_0(r) + U_1(r)\hat{\mathbf{l}} \cdot \hat{\boldsymbol{\sigma}}$. Find the phase shifts $\delta_l^{\pm}$:

a) in the Born approximation;

b) in the quasi-classical approximation.

Calculate also the scattering amplitude in the eikonal approximation, from the partialwave expansion, Eq. (XIII.25).

Solution

The solution of the Schrdinger equation, corresponding to a definite value of the angular momentum squared, $l(l+1)$, the total angular momentum, $j = l \pm 1/2$, and its projection, j_z, has the form:

$$\psi_{kjlj_z} = \tilde{\psi}_{jlj_z} R_{kjl}(r), \quad E = \frac{\hbar^2 k^2}{2m}$$

Here, $\tilde{\psi}_{jlj_z}$ is the spin and angular part of the wavefunction (see Problems 5.24 and 5.25, and note that in this problem its explicit form is not important). Since

$$\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{l}} \tilde{\psi}_{jlj_z} = \left[j(j+1) - l(l+1) - \frac{3}{4} \right] \tilde{\psi}_{jlj_z}$$

then we note that the radial Schrdinger equation for R_{kjl} has the same form as in the case of a spinless particle with the angular momentum l in the potential

$$U_1^{\pm}(r) = U_0(r) \pm \left(l + \frac{1}{2} \mp \frac{1}{2} \right) U_1(r)$$

The upper and lower signs correspond to the values $j = l \pm 1/2$. Replacing the potential $U(r)$ by $U_1^{\pm}$in Eqs. (XIII.12-XIII.14) determines the phase shifts, $\delta_l^{\pm}$, in expansions (XIII.25). Therefore the sought-after generalization of Eq. (XIII.14) has the form:

$$\delta_l^{\pm} \approx -\frac{m}{2\hbar v} \int\limits_{-\infty}^{\infty} \left\{ U_0 \left(\sqrt{\rho^2 + z^2} \right) \pm k\rho U_1 \left(\sqrt{\rho^2 + z^2} \right) \right\} dz, \quad l = \rho k \gg 1$$

Using this relation and Eq. (XIII.25), just as in the case of spinless particles, we can obtain expressions for the invariant amplitudes A and B in the eikonal approximation. It is important to remember that

$$\sin\theta P_l'(\cos\theta) \approx -\frac{\partial}{\partial\theta} J_0(l\theta) = l J_1(l\theta); \quad l \gg 1, \quad \theta \ll 1$$

The scattering amplitude operator (i.e., a matrix function in the spin space) in the eikonal approximation has the following simple form:

$$\hat{f} = \frac{ik}{2\pi} \iint \left\{ 1 - \exp\left\{ 2i\hat{\delta}\left(\mathbf{k}_0, \boldsymbol{\rho}\right) \right\} \right\} e^{-i\mathbf{q}\cdot\boldsymbol{\rho}} d^2\rho \tag{1}$$

which becomes physically more transparent if we introduce an operator for the quasiclassical phase-shift (compare to Eq. (XIII.19)):

$$\hat{\delta}\left(\mathbf{k}_0, \boldsymbol{\rho}\right) = -\frac{m}{2\hbar v} \int\limits_{-\infty}^{\infty} \left\{ U_0(\boldsymbol{\rho}, z) + U_1(\boldsymbol{\rho}, z) \left[\boldsymbol{\rho} \times \mathbf{k}_0\right] \cdot \hat{\boldsymbol{\sigma}} \right\} dz \tag{2}$$

Using the identity

$$\exp\{i\alpha\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{\nu}\} = \cos\alpha + i\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{\nu} \sin\alpha, \text{ where } \boldsymbol{\nu}^2 = 1$$

it is easy to obtain the eikonal expressions for amplitudes A and B in Eq. (XIII.22).

GKKG.13.64

In the case of a spin- 1/2 particle colliding with a spinless particle, find a relation between the scattering amplitude in the helicity representation (see Problem 5.20) and the invariant functions A and B in Eq. (XIII.22).

Solution

Let the plane, where the scattering occurs, be the plane (x, z), where the z axis is directed along momentum $\mathbf{p}_0$ of the particle with spin $s = 1/2$ in the center-ofinertia system before the collision. We have $\mathbf{p}_0 = (0, 0, p)$, $\mathbf{p} = (p\sin\theta, 0, p\cos\theta)$, and $\boldsymbol{\nu} = (0, 1, 0)$, so that $\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{\nu} = \hat{\sigma}_y$.

Taking into account the fact that the helical states, φ_λ before the collision and χ_μ after the collision, are described by the spinors (see Problem 5.20):

$$\varphi_{1/2} = \begin{pmatrix}1\\0\end{pmatrix}, \quad \varphi_{-1/2} = \begin{pmatrix}0\\1\end{pmatrix}; \quad \chi_{1/2} = \begin{pmatrix}\cos(\theta/2)\\ \sin(\theta/2)\end{pmatrix}$$
$$\chi_{-1/2} = \begin{pmatrix}-\sin(\theta/2)\\ \cos(\theta/2)\end{pmatrix}$$

we find the helical amplitudes $f_{\lambda\mu} = \chi^*_\mu \hat{f} \varphi_\lambda$:

$$f_{1/2,1/2} = f_{-1/2,-1/2} = \cos(\theta/2)\cdot A - \sin(\theta/2)\cdot B$$
$$f_{1/2,-1/2} = f_{-1/2,1/2} = -\sin(\theta/2)\cdot A - \cos(\theta/2)\cdot B$$

GKKG.13.65

Upon the collision of two spinless particles, a reaction occurs and two particles are created, one of which has spin $s = 1$, and the other $s = 0$. The intrinsic parities of all particles are positive.

Using the vector representation (see Problem 5.26) to describe the spin states of the particle with $s = 1$, prove that the spin structure of the amplitude for the reaction considered is described by the expression:

$$\langle f|\hat{|}|i\rangle = \mathbf{a}^* \cdot [\mathbf{p}_0 \times \mathbf{p}_1]\, f(E,\theta)$$

where $\mathbf{a}$ is the spin function, and $\mathbf{p}_0$ and $\mathbf{p}_1$ are momenta before and after the collision.
Present a partial-wave expansion of $f(E,\theta)$.
Also determine the spin structure of the amplitude in the case, where the particle with spin $s = 1$ has negative intrinsic parity.

Solution

The wavefunction describing the relative motion of the colliding particles at large distances has the form:

$$e^{ikz} \approx \sum_l i^l (2l+1) P_l(\cos\theta) \frac{1}{2kr} \left\{ e^{-i(kr-\pi l/2)} - e^{i(kr-\pi l/2)} \right\}$$

The term $i^l(2l+1)P_l(\cos\theta)e^{-i(kr-\pi l/2)}/2kr$ of this sum describes the state of the colliding particles (before interaction) with angular momentum $l = 1$, parity $I_l = (-1)^l$, and zero projection of the angular momentum onto the z axis (directed along the momentum $\mathbf{p}_0 = \hbar\mathbf{k}$), i.e., $j_z = l_z = 0$. The particles appearing in this reaction channel, are described (when the separation between them, r_1, is large) by the following outgoing wave:

$$\eta_l(E) \mathbf{\Phi}_{j=l,I_l,j_z=0}(\mathbf{n}_1) \frac{1}{r_1} e^{ik_1 r_1}, \quad \mathbf{n}_1 = \frac{\mathbf{r}_1}{r_1} \tag{1}$$

$\mathbf{\Phi}_{jIj_z}(\mathbf{n})$ describes the spin-angular dependence of the escaping particles. The value of the parameter η_l is determined by the intensity of the interaction. To determine the explicit form of $\mathbf{\Phi}(\mathbf{n}_1)$, we note that the angular momentum of the final state coincides with the initial one, l. Indeed, for total angular momentum $j = l$ and spin $s = 1$, the angular momentum could only take the values $l' = l, l \pm 1$. With the parity of the states accounted for, it follows that $l' = l$ (and $l \neq 0$). Thus,

$$\mathbf{\Phi}_{lI_l0}(\mathbf{n}_1) = \sum_{m=0,\pm1} C^{l0}_{lm,1,-m} Y_{lm} Y_{lm}(\mathbf{n}_1) \boldsymbol{\chi}_{-m} \tag{2}$$

Using the explicit form of the spherical functions, Y_{lm}, the components of the vector χ_m (see Problem 3.41), and the Clebsch-Gordan coefficients,

$$Y_{l,\pm1} = \mp i^l \left[\frac{2l+1}{4\pi l(l+1)}\right]^{1/2} \sin\theta P_l'(\cos\theta) e^{\pm i\varphi}$$
$$\chi_{\pm1} = \mp\frac{i}{\sqrt{2}}(1, \pm i, 0); \quad C^{l0}_{l,\pm l,1,\mp1} = \mp(-1)^l \frac{1}{\sqrt{2}}, \quad C^{l0}_{l0,10} = 0$$

we transform Eq. (2) into the form:

$$\mathbf{\Phi}_{lI_l0} = \gamma_l \sin\theta_1 P_l'(\cos\theta_1)(-\sin\varphi_1, \cos\varphi_1, 0)$$

where

$$\gamma_l = (-i)^l \left[\frac{2l+1}{4\pi l(l+1)}\right]^{1/2}$$

Recognizing that the vector with components $\sin\theta_1(-\sin\varphi_1, \cos\varphi_1, 0)$ is equal to $[\mathbf{p}_0 \times \mathbf{p}_1]/p_0 p_1$, and performing a summation over l, we obtain an equation for the vector amplitude of the "scattered" wave, the

coefficient in front of $e^{ik_1 r_1}/r_1$ in the asymptote of the wavefunction for $r_1 \to \infty$ in the reaction channel considered:

$$\mathbf{\Phi}(\mathbf{n}_1) = f(E,\theta)\,[\mathbf{p}_0 \times \mathbf{p}_1]\,, \quad f(E,\theta) = \sum_l \tilde{\eta}_l(E) P_l'(\cos\theta) \tag{3}$$

with $\tilde{\eta}_l(E) = \eta_l(E)\gamma_l/p_0 p_1$. The differential cross-section for this reaction is summed over the spin states, $d\sigma/d\Omega = (v_1/v_B)\,|\mathbf{\Phi}|^2$, where $v_{0,1}$ are the velocities of the particles' relative motion in the initial and final states. The total reaction cross-section is

$$\sigma_r = \sum_l \sigma_{r,l}; \quad \sigma_{r,l} = \frac{v_1}{v_0}\,|\gamma_l|^{-2}\,p_0^2 p_1^2\,|\tilde{\eta}_l|^2 = \frac{v_1}{v_B}\,|\eta_l(E)|^2$$

From the unitarity condition of the S-matrix, a constraint on the partial reaction cross-section follows: $\sigma_{r,l} \le (2l+1)\pi/k_0^2$.

The reaction amplitude for the creation of the particle with $s = 1$ in a specific spin state, described by the polarization vector $\mathbf{a}$, is determined by the expression:

$$\langle f|\hat{f}|i\rangle = (\mathbf{a}^* \cdot \mathbf{\Phi}) = f(E,\theta)\,(\mathbf{a}^* \cdot [\mathbf{p}_0 \times \mathbf{p}_1]) \tag{4}$$

This was evident before (and does not really require the preceding calculation) from the fact that the reaction amplitude is a scalar quantity. Indeed, it is the only possible scalar combination which could be formed from the vectors $\mathbf{p}_0, \mathbf{p}_1$, and $\mathbf{a}$ (due to the superposition principle, the polarization vector must enter linearly). We should take into account that $\mathbf{a}$ is an axial vector (or pseudo-vector), since under inversion, $\hat{I}\mathbf{a} = +\mathbf{a}$, due to the positive intrinsic parity of the particle with $s = 1$. Let us also note that according to Eq. (4), the particle with $s = 1$, that is created in the reaction considered, becomes linearly polarized in the direction perpendicular to the reaction plane (the spin projection on this direction has a definite value, equal to zero).

In the case of a reaction when the particle with spin $s = 1$ has negative intrinsic parity, its polarization vector, $\mathbf{v}$, is a polar vector (since under inversion $\hat{I}\mathbf{v} = -\mathbf{v}$). So now, from the condition that the transition amplitude is a scalar, it follows that its spin structure has the form: [364]

$$\langle f|\hat{f}|i\rangle = \mathbf{v}^* \cdot \{f_1(E,\theta)\mathbf{p}_0 + f_2(E,\theta)\mathbf{p}_1\} \tag{5}$$

The appearance of the two invariant amplitudes, $f_{1,2}$, is connected with the fact that for a given angular momentum, l, of the colliding particles, the angular momentum of the particles in the final state could take two values: $l' = l \pm 1$.

GKKG.13.66

A spinless particle is scattered from a system of identical spin- 1/2 scattering centers, distributed about the space. Interaction with a single center is described by the expression $\hat{U} = U_0(r) + U_1(r)\hat{\mathbf{l}} \cdot \hat{\boldsymbol{\sigma}}$. Analyze the amplitude and differential scattering cross-section in the Born approximation in the case of non-polarized centers ($\mathbf{P}_n = \mathbf{0}$). Compare to the scattering from the same system of spinless particles.

Solution

In the Born approximation, the scattering amplitude is described by the following expression (compare to Problems 13.7 and 13.8)

$$\hat{f} = \sum_n \{A_n(q) + iB_0(q)\hat{\boldsymbol{\sigma}}_n \cdot \boldsymbol{\nu}\} \exp\{-i\mathbf{q} \cdot \mathbf{a}_n\} \tag{1}$$

Here, $\mathbf{a}_n$ is the radius vector of the nth center, and the real functions $A_0(q)$ and $B_0(q)$ were defined in Problem 13.59.

The differential scattering cross-section, averaged over the initial spin states of the scattering centers and summed over their final spin states, has the form:

$$\left\langle \frac{d\sigma}{d\Omega} \right\rangle = A_0^2(q)\left|\sum_n e^{-i\mathbf{q}\cdot\mathbf{a}_n}\right|^2 + 2A_0(q)B_0(q)\sum_{k\ne n}\mathbf{P}_n \cdot \boldsymbol{\nu}\sin[\mathbf{q}\cdot(\mathbf{a}_n - \mathbf{a}_k)] + NB_0^2(q) + B_0^2(q)\sum_{k\ne n}\overline{(\boldsymbol{\sigma}_n \cdot \boldsymbol{\nu})(\boldsymbol{\sigma}_k \cdot \boldsymbol{\nu})}\cos[\mathbf{q}\cdot(\mathbf{a}_n - \mathbf{a}_k)] \tag{2}$$

where the line means averaging over the initial spin states of the centers. If there is no correlation between the states of single centers, then

$$\overline{(\boldsymbol{\sigma}_n \cdot \boldsymbol{\nu})(\boldsymbol{\sigma}_k \cdot \boldsymbol{\nu})} = (\mathbf{P}_n \cdot \boldsymbol{\nu})(\mathbf{P}_k \cdot \boldsymbol{\nu}), \quad n \ne k$$

[364] Here, as well as in the previous problem, it is important that all other spinless particles that take part in the reaction have positive intrinsic parity (or, more precisely, their product must be positive; in the opposite case, then Eqs. (4) and (5) must be exchanged with one another).

In the case of unpolarized centers, $\mathbf{P}_n = \mathbf{0}$, only the first and third terms in Eq. (2) are different from zero. The first of them is determined by the spin-independent part of the interaction, $U_0(r)$, and has the same form as for the scattering from spinless centers (compare to Problem 13.8). The term $NB_0^2(q)$ is determined by the spin-orbital interaction. Its notable property, is its proportionality to the number of scattering centers, which is due to the lack of coherence between them. This term corresponds to scattering involving a spin-flip (so that we can indicate which particular scattering center was involved in the scattering; therefore, there is no interference).

GKKG.13.67

How to generalize the optical theorem to describe scattering of quantum particles with non-zero spin?

Solution

From the unitarity of the S-matrix, the optical theorem is

$$\mathrm{Im}\langle \mathbf{p}, \alpha | \hat{f} | \mathbf{p}, \alpha \rangle = \frac{k}{4\pi} \sigma_{tot}(\mathbf{p}, \alpha)$$

where $\mathbf{p} = \hbar\mathbf{k}$ is the relative momentum of the colliding particles, and α characterizes their spin state. On the left-hand side of the equation is the imaginary part of the elastic forward scattering amplitude, $\theta = 0$, without change of the particle spin state. On the right-hand side is the total scattering cross-section (including inelastic collisions) for the same spin state.

17.4.6 Problems about analytic properties of the scattering amplitude

(Этот раздел интересен тем, кто хочет общее развитие в теории получить, тем кто хочет применять теорию он очень малополезен.)

GKKG.13.68

Analyze the analytical properties and dispersion relation for the scattering amplitude on a zero-range potential (see Problem 13.20). Consider separately the cases with and without a bound state in the potential. Compare to Eq. (XIII.27).

Solution

The scattering amplitude for a zero-range potential is (see Problem 13.20)

$$f(E) = \frac{1}{-1/a_0 - (i/\hbar)\sqrt{2mE}} \tag{1}$$

As an analytical function of the complex variable E, it has branch points at $E = 0$ and $E = \infty$ and a pole at the point E_0, for which $\sqrt{E_0} = i\hbar a_0/\sqrt{2m}$. Making the branch cut along the real semiaxis, as usual (see Fig. 13.7), and choosing the phase on the upper side of the cut to be equal to $\varphi = 0$, we see that for $a_0 > 0$, pole E_0 is located on the physical sheet and corresponds to a bound state in the zero-range potential (compare to Problem 2.30). When $a_0 < 0$, the pole is located on the unphysical Riemann sheet and corresponds to a virtual level.

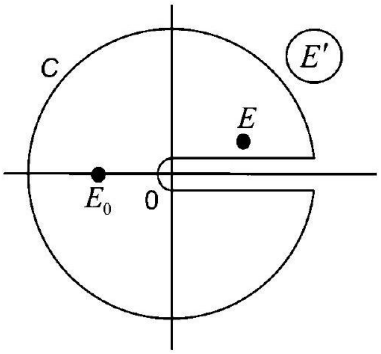


Fig. 13.7

Let us consider the integral over the contour C in Fig. 13.7:

$$\frac{1}{2\pi i}\int\limits_C \frac{f\left(E'\right)dE'}{\left(E'-E\right)} \tag{2}$$

Using Cauchy's theorem, and sending the contour circle radius to infinity, $R_E \to \infty$, in the case of $a_0 > 0$ we obtain:

$$f(E) = -\frac{\hbar^2}{ma_0\left(E-E_0\right)} + \frac{1}{\pi}\int\limits_0^\infty \frac{\operatorname{Im} f\left(E'\right)dE'}{E'-E} \tag{3}$$

We have used the fact that the value of the amplitude jump on the cut (for $E' > 0$) coincides with $2i \operatorname{Im} f\left(E'\right)$ (on the lower side of the cut, $\sqrt{E} = -\sqrt{|E|}$), and that the value of the integral is determined by the contribution of two poles: E and E_0.

In the case $a_0 < 0$, pole E_0 is on the unphysical sheet. It does not contribute to the value of integral (2), and the dispersion relation has a form analogous to (3), but without the pole term.

The dispersion relation in the case of a zero-range potential can be found by direct calculation. Substituting the imaginary part of the scattering amplitude (1), equal to

$$\operatorname{Im} f(E) = \sqrt{\frac{\hbar^2 E}{2m}}\frac{1}{|E_0|+E}, \quad E > 0$$

into the integral in Eq. (3) and integrating, we obtain:

$$\tilde{f}(E) = \frac{1}{\pi}\sqrt{\frac{\hbar^2}{2m}}\int\limits_0^\infty \frac{\sqrt{E'}dE'}{\left(E'-E\right)\left(|E_0|+E'\right)} = \frac{\hbar}{\sqrt{2m}}\frac{1}{\sqrt{|E_0|}-i\sqrt{E}}$$

In the case $a_0 < 0$ (without a bound state), this coincides with the scattering amplitude, Eq. (1). In the case $a_0 > 0$, we obtain the scattering amplitude after adding, according to Eq. (3), the pole term.

The dispersion relations found differ from Eq. (XIII.27) by the absence of the term $f_B \propto \int UdV$. This has a simple explanation. A zero-range potential can be obtained from a potential of finite radius, R, by passage to the limit $R \to 0$ for which $U_0R^2 = \text{const}$, so that we would have $f_B \propto U_0R^3 \to 0$. In a finite-range potential, the scattering amplitude in the limit $E \to \infty$ coincides with the Born one. In order to have a condition as in Eq. (2), we subtract f_B from f on a circle of the finite radius (for a zero-range potential, the scattering amplitude goes to zero for $E \to \infty$).

In conclusion, we note that the residue at the point $E = E_0$ in Eq. (3) is equal to $-\hbar^2/ma_0 = -\hbar^2A^2/2m$. The coefficient $A = \sqrt{2/a_0} = \sqrt{2\kappa_0}$ coincides with the normalization coefficient in the wavefunction,

$$\psi_0 = A\frac{\exp\left\{-\kappa_0 r\right\}}{\sqrt{4\pi}r}$$

of the bound state in the zero-range potential (see Problem 4.10), in accordance with Eqs. (XIII.27) and (XIII.28).

GKKG.13.69

Using the dispersion relation, prove that there is the following restriction on the energy-dependence of the particle-scattering cross-section in a repulsive potential, $U(r) \geq 0$:

$$\int\limits_0^\infty \frac{\sigma(E)}{\sqrt{E}}dE < 4\pi^2\frac{\sqrt{2m}}{\hbar}\int\limits_0^\infty r^2U(r)dr$$

Solution

Since according to the optical theorem, $\operatorname{Im} f(E,0) = k\sigma(E)/4\pi$, then from the dispersion relation, Eq. (XIII.27), for energy $E = 0$, it follows that

$$f(E=0) = -\frac{m}{2\pi\hbar^2}\int U(r)dV + \frac{\sqrt{2m}}{4\pi^2\hbar}\int\limits_0^\infty \frac{\sigma(E)dE}{\sqrt{E}} \tag{1}$$

Here we have also used the fact that in the repulsive potential $U(r) \geq 0$, there are no bound states. Due to the fact that in such a potential we have $f(E=0) < 0$ (see Problems 13.16 and 13.31), we immediately obtain the inequality given in the problem condition.

Let us note that in the case of a "weak" potential, $U_0 \ll \hbar^2/mR^2$, the inequality considered becomes obvious (since $f \propto U_0$, while $\sigma \propto U_0^2$) and is well-fulfilled. But for
a "strong" repulsive potential, [365] $U_0 \gg \hbar^2/mR^2, |f_B| \gg |f(E=0)|$, and the terms of the inequality are approximately the same:

$$\int_0^\infty \frac{\sigma(E)}{\sqrt{E}} dE \approx 4\pi^2 \frac{\sqrt{2m}}{\hbar} \int_0^\infty U(r) r^2 dr \tag{2}$$

In conclusion, we note that from relation (1), obtained in Problem 13.16 by another method, it follows that in a repulsive potential the Born approximation for $E = 0$ greatly overestimates the scattering cross-section.

GKKG.13.70

Prove the relation

$$\int_0^\infty \frac{\sigma(E)}{\sqrt{E}} dE < \pi \sqrt{\frac{2\pi\hbar^2}{m}\sigma(0)}$$

for the scattering in an attractive potential, $U(r) \leq 0$, where there are no bound states (the well is not deep enough). Here $\sigma(0) = 4\pi a_0^2$ is the scattering cross-section for $E = 0$. In what case both sides of the inequality are close?

Solution

Because there are no bound states in the attractive potential, relation (1) from the previous problem is still valid. Now, however, all three terms in it are positive. So in particular, the result from Problem 13.16 follows for the attractive potential. Then the inequality from the problem condition in the case of a "weak" potential must be conservatively valid (compare to the previous problem). When this potential approaches the "critical" one, where a bound state appears, we obtain $f(E = 0) \to \infty$, so that $f(E = 0) \gg f_B$. The values of both inequality parts are close to one another, so that

$$\int_0^\infty \frac{\sigma(E)}{\sqrt{E}} dE \approx \pi \sqrt{\frac{2\pi\hbar^2}{m}\sigma(0)} \tag{1}$$

However, this relation in the case of a "shallow" (real or virtual) s-level in the potential is evident. According to Eq. (XIII.16) in the region of small energies, the scattering cross-section is anomalously large.

$$\sigma(E) \approx \frac{2\pi\hbar^2}{m\,(E + \varepsilon_0)}, \quad \varepsilon_0 \ll \frac{\hbar^2}{mR^2}$$

[365] As an example, for a square potential barrier of radius R, for $U_0 \to \infty$, we also have $|f_B| \to \infty$, but $f(E = 0) = -R = \text{const}$.
This region has the dominant contribution to the value of the integral; by calculating it, we prove relation (1).

GKKG.13.71

Using only the condition of unitary and the dispersion relation (for $q^2 \neq 0$), it is possible to reconstruct [366] the scattering potential in a series over powers of the interaction potential, by the known expression for scattering amplitude in the Born approximation.

As an example, prove that the calculation of the second-order perturbative amplitude for $q^2 = 0$ reproduces the result of perturbation theory over the potential, based on the Schrdinger equation (see Problem 13.10).

Solution

The iteration procedure for the calculation of scattering amplitude $f = \sum_n f^{(n)}$ is the following. First, by the known amplitude of first approximation, $f^{(1)} = f_B$, we can use the unitarity condition, Eq. (XIII.26), to find the imaginary part of the second, order amplitude, [367] $\operatorname{Im} f^{(2)}\left(E, q^2\right)$. Then, using the dispersion relation for $q^2 \neq 0$ (analogous to Eq. (XIII.27)), we can find the entire amplitude, $f^{(2)}$. Higher-order approximation terms are calculated in the same way.

In particular, for the value $q^2 = 0$ we easily find

$$f^{(2)}\left(E, q^2=0\right)=\frac{1}{4\pi}\int\limits_0^\infty \frac{dE'}{\sqrt{E'}\,(E'-E)}\int\limits_0^{4E'} f_B^2(x)dx \tag{1}$$

The imaginary part of the scattering amplitude with the help of the optical theorem is expressed in terms of the scattering cross-section in the Born approximation. For simplicity, we use the system of units $\hbar = 2m = 1$. With this, $E = k^2$. The Born amplitude, f_B, is written in the form $f_B\left(q^2\right)$.

On the other hand, in the 2nd order of perturbation theory according to the result from Problem 13.10, we have:

$$f^{(2)}\left(E, q^2=0\right)=\frac{1}{2\pi^2}\int \frac{f_B^2\left(\left(k_0-\kappa\right)^2\right)}{\kappa^2-E}d^3\kappa = \frac{1}{2\pi}\int\limits_0^\infty \frac{\kappa d\kappa}{\sqrt{E}\,(\kappa^2-E)}\int\limits_{(\kappa-\sqrt{E})^2}^{(\kappa+\sqrt{E})^2} f_B^2(x)dx \tag{2}$$

[366] Let us emphasize that the Schrdinger equation is not used here.

[367] Here, in principle, the relation obtained gives the imaginary part of the amplitude also for the unphysical values of energy $0 < E < \hbar^2 q^2/8m$.

To prove that Eqs. (1) and (2) are actually the same, we make the following transformations (note that their equivalence becomes obvious in the $E \to 0$ limit, if we integrate Eq. (1) by parts): First, we divide the "internal" integral in Eq. (2) into two, with the point $x = 0$ as one of the integration limits. Then, in the first of two terms that appear as a result, use the substitution $2\kappa' = \kappa + \sqrt{E}$, while in the second, use $2\kappa' = \kappa + \sqrt{E}$. In the resulting integrals over κ', again divide the integration domains into two: from 0 to ∞ and from 0 to $\pm\sqrt{E}/2$. The contributions of the latter integration domains cancel each other out, while the sum of the contributions of the former reproduces (after the substitution, $E' = (\kappa')^2$) Eq. (1).

GKKG.13.72 Upper bound for the amplitude

Consider the interaction for partial waves with $l \geq L_0 \equiv kR \gg 1$ to be negligibly small, and obtain the upper bound for the scattering amplitude of spinless particles at high energies for different scattering angles.

Solution

In the scattering amplitude expansion over partial waves, Eq. $f(k,\theta) = \sum\limits_{l=0}^{\infty}(2l+1)\varphi_l(E)P_l(\cos\theta)$; $\varphi_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k(\cot\delta_l - i)}$, we have the inequality $|\varphi_l| \leq 1/k$, so that in accordance with the problem condition we obtain:

$$|f(k,\theta)| \leq \frac{1}{k}\sum_{l=0}^{L_0}(2l+1)\,|P_l(\cos\theta)| \tag{1}$$

Replacing the summation by integration, for angles $\theta = 0$ and $\theta = \pi$ we find:

$$|f| \leq \frac{L_0^2}{k} = kR^2, \quad \theta = 0;\pi \tag{2}$$

For scattering angles, $\theta \neq 0, \pi$, we have:

$$|P_l(\cos\theta)| \leq \left(\frac{2}{\pi l \sin\theta}\right)^{1/2}$$

and so we obtain:

$$|f(\theta)| \leq \frac{4}{3}\left(\frac{2}{\pi\sin\theta}\right)^{1/2} R(kR)^{1/2} \tag{3}$$

Note that due to the Legendre polynomials oscillation for $\theta \neq 0$, such a restriction for arbitrary scattering angle is too weak and conservatively valid. Indeed, the restriction

[368] In Problems 13.72-13.75, general constraints on the interaction amplitudes and cross-sections for large energies are discussed. These restrictions are connected, basically, with the possibility of neglecting interaction at distances that are larger than the radius of the potential, R. This situation occurs frequently in elementary particle physics. Here, the effective interaction radius increases with energy, but not faster than $\propto \ln(E/E_0)$ (see Problem 13.53). The necessity of using relativistic kinematics is practically not reflected in the results. on the value of total elastic scattering cross-section which follows from inequality (3), $\sigma_{el} = \int |f|^2 d\Omega \leq CR^2 kR$, is uninteresting, since $\sigma_{el} \leq \sigma_{tot} \leq 4\pi R^2$ and $kR \gg 1$.

GKKG.13.73 lower bound on the cross-section

Under the conditions of the previous problem, obtain the lower bound on the value of the elastic scattering cross-section, σ_{el}, of fast particles for a given value, σ_{tot}, of the total collision cross-section.

Solution

From the expressions for partial cross-sections (total and elastic cross-sections),

$$\sigma_{\text{tot}}^{(l)} = 2\pi(2l+1)\frac{1}{k^2}\left(1 - \operatorname{Re} S_l\right)$$
$$\sigma_{el}^{(l)} = \pi(2l+1)\frac{1}{k^2}\left|1 - S_l\right|^2 = \pi(2l+1)\frac{1}{k^2}\left(1 - 2\operatorname{Re} S_l + |S_l|^2\right)$$

it follows that for a given value of $\sigma_{\text{tot}}^{(l)}$, the quantity $\sigma_{el}^{(l)}$ is minimal for $\operatorname{Im} S_1 = 0$. Thus,

$$\sigma_{el} = \sum_l \sigma_{el}^{(l)} \geq \tilde{\sigma}_{el} = \frac{\pi}{k^2}\sum_{l=0}^{L_0}(2l+1)\left(1-\alpha_l\right)^2$$

where $\alpha = \operatorname{Re} S_l$. To find the minimum value of $\tilde{\sigma}_{el}$ as a function of variables α_l for the given $\sigma_{tot} = \sum\limits_l \sigma_{tot}^{(l)}$, we use Lagrange's method of undetermined multipliers and introduce $A(\alpha_l) = \tilde{\sigma}_{el} - \lambda\sigma_{tot}$. From the extremality conditions (now all variables α_l could be varied independently) for $A(\alpha_l)$, we find that $\alpha_l = \text{const} = \alpha$ (no dependence on l). Replacing summation over l by integration and excluding α from the expressions for σ_{el} and σ_{tot}, we obtain the inequality

$$\sigma_{el} \geq \min \tilde{\sigma}_{el} = \frac{1}{4\pi R^2}\sigma_{tot}^2 \tag{1}$$

As mentioned in Problem 13.53, in the theory of strong elementary particle interactions there is a restriction on the possible growth of the interaction radius R with increase in energy:

$$R \leq R_0 \ln\frac{E}{E_0} \text{ for } E \to \infty \tag{2}$$

From this, inequality (1) takes the form:

$$\sigma_{el}(E) \geq C\frac{\sigma_{tot}^2(E)}{\ln^2(E/E_0)} \tag{3}$$

GKKG.13.74 Upper bound for Re(f)

For large energies, find the upper bound for the real part of the amplitude for elastic forward scattering, $\theta = 0$, assuming that the total collision cross-section is known and that particle interaction is negligibly small for distances above R. What is the restriction for $|f(E, \theta = 0)|$?

Solution

Denoting $S_l = |S_l|\, e^{2i\delta_l}$ for the partial amplitudes in Eq. $f(k,\theta) = \sum\limits_{l=0}^{\infty}(2l+1)\varphi_l(E)P_l(\cos\theta)$; $\varphi_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k(\cot\delta_l - i)}$, we have the following expressions:

$$\operatorname{Im}\varphi_l = \frac{1}{2k}\left(1 - |S_l|\cos 2\delta_l\right), \quad \operatorname{Re}\varphi_l = \frac{1}{2k}|S_l|\sin 2\delta_l$$

For this value of $\operatorname{Im}\varphi_l$, the value of $|\operatorname{Re}\varphi_l|$ is maximum when $|S_l| = 1$. In this case, inelastic scattering is absent and $\sigma_{tot} = \sigma_{el}$. So, writing $\operatorname{Im}\varphi_l = (1-\alpha_l)/2k$, we obtain

$$|\operatorname{Re} f(E,0)| \le \sum_l (2l+1)\,|\operatorname{Re}\varphi_l| \le \frac{1}{2k}\sum_{l=0}^{L_0}(2l+1)\sqrt{1-\alpha_l^2}$$

Using the method from the previous problem, we obtain the following restriction on the real part of the elastic forward scattering amplitude for the total scattering cross-section:

$$|\operatorname{Re} f(E,0)| \le \frac{1}{2\sqrt{\pi}}\sqrt{\sigma_{tot}}kR\left(1-\frac{\sigma_{tot}}{4\pi R^2}\right)^{1/2} \le \frac{1}{2\sqrt{\pi}}\sqrt{\sigma_{tot}}kR \tag{1}$$

So, taking into account the fact that $\sigma_{tot} \le 4\pi R^2$ and the restriction on interaction radius growth with increase in energy (see the previous problem), we obtain

$$|f(E,0)| \le Ck\sqrt{\sigma_{tot}(E)}\ln\frac{E}{E_0} \tag{2}$$

Here, we used the optical theorem.
As mentioned before, restriction (1) suggests the absence of inelastic processes. Analogously (using Lagrange's method of undetermined multipliers), we can obtain a less strict restriction on the scattering amplitude for given values of both total, σ_{tot}, and inelastic, σ_{inel} , collision cross-section.

GKKG.13.75

Prove that for large energies, the derivative with respect to θ at $\theta = 0$ of the imaginary part of the elastic scattering amplitude satisfies the following inequalities:

$$\frac{\sigma_{tot}}{32\pi} \le -\frac{d}{dq^2}\ln \operatorname{Im} f(E,q)\bigg|_{q=0} \le \frac{R^2}{4}, \quad q = 2k\sin\left(\frac{\theta}{2}\right)$$

where σ_{tot} is the total collision cross-section and R is the interaction radius. (At distances larger than R, the interaction is negligibly small.)
Verify explicitly that these inequalities are indeed satisfied by the diffraction scattering amplitude from Problem 13.57.

Solution

Since for the Legendre polynomial, $P_l'(1) = l(l+1)/2$, then using the scattering amplitude expansion over partial waves, Eq. $f(k,\theta) = \sum_{l=0}^{\infty}(2l+1)\varphi_l(E)P_l(\cos\theta)$; $\varphi_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k(\cot\delta_l - i)}$, for high energies we obtain

$$\frac{d}{d\cos\theta}\operatorname{Im} f(E,\theta)\bigg|_{\theta=0} \approx \sum_l l^3 \operatorname{Im}\varphi_l \tag{1}$$

Using the fact that $\operatorname{Im}\varphi_l \le 1/k$, we see that for a given total scattering cross-section, and so the imaginary part of the scattering amplitude, $\operatorname{Im} f(E,0)$ (due to the optical theorem), the sum (1) takes the minimum value when

$$\operatorname{Im}\varphi_l = \begin{cases} \frac{1}{k}, l \le L_1 \\ 0, l > L_1 \end{cases} \tag{2}$$

The value of L_1 is determined by the total cross-section:

$$\sigma_{tot} = \frac{4\pi}{k}\sum_l (2l+1)\operatorname{Im}\varphi_l \approx \frac{8\pi}{k^2}\sum_{l=0}^{L_1} l$$

Replacing summation over l by integration, we obtain $L_1^2 = k^2\sigma_{tot}/4\pi$ and the following restriction:

$$-\frac{d}{dq^2}\operatorname{Im} f\left(E,q^2\right)\bigg|_{q^2=0} \ge \frac{1}{128\pi^2}k\sigma_{tot}^2(E) \tag{3}$$

We emphasize that relations (2) correspond to the "saturation" of the total scattering cross-section by the lower partial waves. Here $\sigma_{tot} = \sigma_{el}$ (there are no inelastic processes), and moreover, for $l \le L_1$ all of the phases are $\delta_l = \pi/2$, so that restriction (3) must be fulfilled conservatively.
In the same way, we note that the sum in (1) takes the maximum value in the case when total scattering cross-section is saturated by the higher partial waves and

$$\operatorname{Im}\varphi_l = \begin{cases} 0, l < L_2 \\ \frac{1}{k}, L_2 \le l \le L_0 = kR \end{cases}$$

We obtain the following restriction (now from above):

$$-\left.\frac{d}{dq^2}\operatorname{Im} f\left(E,q^2\right)\right|_{q^2=0} \leq \frac{kR^2\sigma_{tot}}{16\pi}\left(1-\frac{\sigma_{tot}}{8\pi R^2}\right) \leq \frac{kR^2\sigma_{tot}}{16\pi} \tag{4}$$

As an example, consider an impenetrable sphere of the radius R (see Problems 13.57 and 13.90). The diffraction scattering amplitude is

$$f_{difr} = i\frac{kR}{q}J_1(qR)$$

The restrictions of the problem condition, which are the direct result of relations (3) and (4), take the form of the following inequality (after cancelling out the factor $R^2/4$): $1/3 < 1/2 < 1$.

In conclusion, we should emphasize that, as mentioned above, restrictions on (3) and (4) assume the absence of inelastic processes. Using the method of Lagrange multipliers, just as in Problem 13.73, we can obtain weaker restrictions when the values of both total and inelastic collision cross-sections are given independently.

GKKG.13.76

Prove unitarity of the scattering amplitude in the eikonal approximation.

Solution

The eikonal approximation assumes that only small scattering angles are important. For these angles, the right-hand part of relation (XIII.26) with the eikonal expression for the amplitude, Eq. (XIII.18), taken into account could be transformed to the form:

$$\frac{ik}{2\pi}\iint \left[S^*(\boldsymbol{\rho})-1\right]\left[S(\boldsymbol{\rho})-1\right]\exp\left\{-i\mathbf{q}_\perp\cdot\boldsymbol{\rho}\right\}d^2\rho \tag{1}$$

To perform the integration over angles which leads to Eq. (1), we use the relations:

$$\mathbf{k}-\mathbf{k}_0 \approx \mathbf{q}_\perp, \quad \mathbf{k}'-\mathbf{k}_0 \approx \mathbf{q}'_\perp, \quad \mathbf{k}'-\mathbf{k} \approx \mathbf{q}'_\perp-\mathbf{q}_\perp, \quad d\Omega' \approx \frac{1}{k^2}d^2q'_\perp$$

Although $q_\perp, q'_\perp \ll k$, due to the fast decrease of the integrand, we can integrate over $q_\perp$ in infinite limits. Using Eq. (XIII.19) for $S(\rho)$, we find the relation:

$$\left[S^*(\boldsymbol{\rho})-1\right]\left[S(\boldsymbol{\rho})-1\right] = \left[1-S(\boldsymbol{\rho})\right]-\left[S^*(\boldsymbol{\rho})-1\right]$$

So now Eq. (1) takes the form $f\left(\mathbf{k},\mathbf{k}_0\right)-f^*\left(\mathbf{k}_0,\mathbf{k}\right)$, which proves the unitarity of the scattering amplitude in the eikonal approximation. In particular, according to the optical theorem, the expression for the scattering cross-section of fast particles, discussed in Problem 13.51, follows.

17.4.7 Problems about scattering on composite particles, inelastic collisions

(тут какая-то очень профессиональная теория, можно не изучать это заранее, потому что это однозначно выходит за рамки минимальной подготовки)

ПТФ-13.з3. Рассеяние на двухатомной молекуле

Смоделируем двухатомную полярную молекулу потенциалом вида $V(\mathbf{r}) = V_0(\mathbf{r}+\frac{\mathbf{R}}{2}) + V_0(\mathbf{r}-\frac{\mathbf{R}}{2})$ (вектор $\mathbf{R}$ соединяет два атома, а $V_0(\mathbf{r})$ представляет собой потенциал рассеяния на отдельном атоме). В рамках Борновского приближения, свяжите дифференциальное сечение рассеяния на такой молекуле с сечением на отдельном атоме. Считая различные ориентации молекулы равновероятными, усредните по ним результат. Как связаны полные сечения рассеяния для случая медленных ($kR \ll 1$) и достаточно быстрых ($ka \sim 1$, но $R \gg a$, где a – характерный масштаб потенциала $V_0(r)$) частиц?

Solution.

$$f(\mathbf{n},\mathbf{n}') = -\frac{m}{2\pi\hbar}\tilde{V}_{\mathbf{k}-\mathbf{k}'} = -\frac{m}{2\pi}\int d^3\mathbf{r}V(\mathbf{r})e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{r}} =$$
$$= -\frac{m}{2\pi}\int d^3\mathbf{r}\left(V_0\left(\mathbf{r}+\frac{\mathbf{R}}{2}\right)+V_0\left(\mathbf{r}-\frac{\mathbf{R}}{2}\right)\right)e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{r}} =$$
$$= -\frac{m}{2\pi}\int d^3\mathbf{r}\left(V_0(\mathbf{r})e^{i(\mathbf{k}-\mathbf{k}')\frac{\mathbf{R}}{2}}+V_0(\mathbf{r})e^{-i(\mathbf{k}-\mathbf{k}')\frac{\mathbf{R}}{2}}\right)e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{r}} =$$
$$= 2f_0(\mathbf{n},\mathbf{n}')\cos\left(\frac{(\mathbf{k}-\mathbf{k}')\mathbf{R}}{2}\right)$$

$f_0(\mathbf{n},\mathbf{n}') := -\frac{m}{2\pi}\tilde{V}_{0\mathbf{k}-\mathbf{k}'} = -\frac{m}{2\pi}\int d^3\mathbf{r}V_0(\mathbf{r})e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{r}}$.

$$d\sigma = |f(\mathbf{n},\mathbf{n}')|^2 d\Omega_{\mathbf{n}'}, \qquad d\sigma_0 = |f_0(\mathbf{n},\mathbf{n}')|^2 d\Omega_{\mathbf{n}'}$$

$$d\sigma = 4\cos^2\left(\frac{(\mathbf{k}-\mathbf{k}')\mathbf{R}}{2}\right)d\sigma_0$$

Усредним величину $\frac{d\sigma}{d\sigma_0}$ по различным ориентациям молекулы.

$$\left\langle\frac{d\sigma}{d\sigma_0}\right\rangle = \frac{1}{4\pi}\int 4\cos^2\left(\frac{(\mathbf{k}-\mathbf{k}')\mathbf{R}}{2}\right)d\Omega = \frac{4\cdot 2\pi}{4\pi}\int\limits_0^\pi \cos^2\left(\frac{|\mathbf{k}-\mathbf{k}'|R\cos\theta}{2}\right)\sin\theta d\theta =$$
$$= \left\langle\frac{d\sigma}{d\sigma_0}\right\rangle = 2\left(1+\frac{\sin(|\mathbf{k}-\mathbf{k}'|R)}{|\mathbf{k}-\mathbf{k}'|R}\right)$$

$|\mathbf{k}| = |\mathbf{k}'| \to |\mathbf{k}-\mathbf{k}'| = \sqrt{k^2+k'^2-2kk'\cos\alpha} = \sqrt{2k^2(1-\cos\alpha)} = 2k\sin\frac{\alpha}{2}$,

$$\left\langle\frac{d\sigma}{d\sigma_0}\right\rangle = 2\left(1+\frac{\sin(2k\sin\frac{\alpha}{2}R)}{2k\sin\frac{\alpha}{2}R}\right)$$

Найдём связь между полными сечениями:

$$\langle\sigma\rangle = \int 2\left(1+\frac{\sin(2k\sin\frac{\alpha}{2}R)}{2k\sin\frac{\alpha}{2}R}\right)|f_0(\mathbf{n},\mathbf{n}')|^2\sin\alpha d\alpha d\varphi = 2\left(\langle\sigma_0\rangle+\int\frac{\sin(2k\sin\frac{\alpha}{2}R)}{2k\sin\frac{\alpha}{2}R}|f_0(\mathbf{n},\mathbf{n}')|^2\sin\alpha d\alpha d\varphi\right)$$

• Случай медленных частиц ($kR \ll 1$).

$$\langle\sigma\rangle \approx 2\left(\langle\sigma_0\rangle+\int|f_0(\mathbf{n},\mathbf{n}')|^2\sin\alpha d\alpha d\varphi\right) = 4\langle\sigma_0\rangle$$

• Случай достаточно быстрых частиц ($ka \sim 1$, $R \gg a$). Подынтегральное выражение быстро осциллирует, поэтому

$$\langle\sigma\rangle \approx 2\langle\sigma_0\rangle$$

GKKG.13.77

Prove that the amplitude of elastic scattering of an electron with an atom (the composite system) in the Born approximation coincides with the amplitude of electron scattering from a static local potential $U(\mathbf{r})$, if we neglect exchange effects. [369] Find its physical meaning. Compare to Problems 13.4-6.

Solution

The interaction between the incident electron and the atom has the form ($\mathbf{r}_a$ are radius vectors of the atomic electrons):

$$U(\mathbf{r},\{\mathbf{r}_a\}) = -\frac{Ze^2}{r}+\sum_a\frac{e^2}{|\mathbf{r}-\mathbf{r}_a|}$$

The electron's elastic scattering amplitude on the atom in the Born approximation, if we neglect exchange effects (which play a role of higher-order corrections) is described by an expression similar to Eq. (XIII.6):

$$f_B = -\frac{m}{2\pi\hbar^2}\int \psi_0^*(\xi_a)\, e^{-i\mathbf{k}\cdot\mathbf{r}} U(\mathbf{r}, \{\mathbf{r}_a\})\, e^{i\mathbf{k}_0\cdot\mathbf{r}}\psi_0(\xi_a)\, dV d\tau\xi \tag{1}$$

Integration over τ_ξ also includes a summation over the spin variables of the atomic electrons. Performing the integration over ξ_a and also examining the "potential",

$$\varphi_{at} = \int\left(\frac{Ze}{r} - \sum_a \frac{e}{|\mathbf{r}-\mathbf{r}_a|}\right)|\psi_0(\xi_a)|^2\, d\tau \tag{2}$$

which gives the mean value of the electrostatic potential maintained by the atom, we see that expression (1) has the form of Eq. (XIII.6) for the scattering amplitude in the Born approximation, with the local potential $U(\mathbf{r}) = -e\varphi_{at}(\mathbf{r})$. Applications are considered in Problems 13.4-13.6.

GKKG.13.78

A polarized electron with $s_z = +1/2$ collides with a hydrogen atom that is in the ground state, where the electron has the opposite value of spin projection, $s_z = -1/2$. In the Born approximation, find the amplitude and cross-section of a spin-flip collision (i.e., the case when $s_z = -1/2$ for a scattered electron, while $s_z = +1/2$ for the atomic
electron), while the atom remains in the ground state. Compare to the case of elastic scattering without spin-flip (see Problem 13.77).

Solution

The system Hamiltonian (with an infinitely heavy proton nucleus) is described by the expression:

$$\hat{H} = \frac{1}{2m}\left(\hat{\mathbf{p}}_1^2 + \hat{\mathbf{p}}_2^2\right) - \frac{e^2}{r_1} - \frac{e^2}{r_2} + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

Spin projections, s_z, for each electron are conserved, and the electrons with $s_z = +1/2$ and $s_z = -1/2$ could be considered as distinguishable particles (anti-symmetrization of the wavefunction is not reflected in the results). So, we denote the electron with $s_z = +1/2$ by e_1 and the electron with $s_z = -1/2$ by e_2. Now we see that the process considered is

$$e_1 + (e_2 p) \to e_2 + (e_1 p) \tag{1}$$

where, the symbol $(e_a p)$ corresponds to the hydrogen atom with electron e_a. We see that this process involves a redistribution of particles, where the initial and final channels of the reaction are different.

Amplitudes of such processes are expressed in terms of matrix elements of the corresponding T-operator, which could be written in two different forms:

$$\hat{T}_1 = V_\alpha + V_\beta \frac{1}{E - \hat{H} + i0} V_\alpha \tag{2a}$$

$$\hat{T}_2 = V_\beta + V_\beta \frac{1}{E - \hat{H} + i0} V_\alpha \tag{2b}$$

Here α and β enumerate reaction channels, $V_{\alpha,\beta}$ describes the interaction in the corresponding channels (α initial, β final channels). Note that although $\hat{T}_1 \neq \hat{T}_2$, reaction amplitudes $\langle\beta|\hat{T}_{1,2}|\alpha\rangle$ coincide.

Further, for the plane waves, $\psi = e^{i\mathrm{pr}/\hbar}$, describing relative motion in each of the two-particle channels [370] we use a probability density that is normalized to unity. The differential cross-section of a process is connected to its element of the T-matrix, $\langle\beta|\hat{T}|\alpha\rangle$, by the expression:

$$\frac{d\sigma}{d\Omega} = \frac{\mu_1\mu_2}{(2\pi)^2\hbar^4}\frac{p_2}{p_1}|\left\langle\beta|\hat{T}|\alpha\right\rangle|^2$$

where $p_{1,2}$ and $\mu_{1,2}$ are the momenta, and the reduced masses for colliding particles in channels α, β; $d\Omega$ is an element of the scattering solid angle in the center-ofmass system. The amplitude of elastic scattering commonly used ($\mu_1 = \mu_2, p_1 = p_2$)

[0] [369] In the Born approximation (for fast particles), the neglect of exchange effects is valid. It is important that the spin state of the free electron, as well as the atomic one, is not changed during collision. Compare to Problem 13.78.

[370] These waves (but not the incoming and outgoing waves), in a product involving the wavefunctions of bound states corresponding to composite particles in the channels (compare to Eq. (3)), appear in the matrix elements, $\langle\beta|\hat{T}|\alpha\rangle$, that determine reaction amplitudes.
is connected to the T-matrix by the relation:

$$f = -\frac{\mu}{2\pi\hbar^2}\langle\alpha|\hat{T}|\alpha\rangle$$

The same relation is valid in the case of inelastic collisions, if $\mu_1 \approx \mu_2, p_1 \approx p_2$.
Using Eq. (2a), we can calculate the amplitude of process (1) to the first order of approximation, i.e., restricting ourselves to the term V_α in $\hat{T}_1$. In this case, $V_\alpha = -e^2/r_1 + e^2/|\mathbf{r}_1 - \mathbf{r}_2|$, and the amplitude of the process considered with electron's spin-flip takes the form:

$$f_{\downarrow\uparrow,\uparrow\downarrow} = -\frac{m}{2\pi\hbar^2}\int \psi_0^*(r_1)\, e^{-i\mathbf{p}_2\cdot\mathbf{r}_2/\hbar}\left[\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|} - \frac{e^2}{r_1}\right] e^{i\mathbf{p}_1\cdot\mathbf{r}_1/\hbar}\psi_0(r_2)\, dV_1 dV_2 \tag{3}$$

where $\mathbf{p}_{1,2}$ are momenta of the electron becoming bound and of the scattered electron, and $\psi_0(r)$ is the wavefunction of the hydrogen atom in the ground state. In the momentum representation (below we use atomic units $e = \hbar = m = 1$),

$$U(r) = \frac{1}{r} = \int e^{i\boldsymbol{\kappa}\cdot\mathbf{r}}\tilde{U}(\kappa)d^3\kappa, \quad \psi_0(r) = \frac{1}{\sqrt{\pi}}e^{-r} = \frac{1}{(2\pi)^{3/2}}\int e^{i\boldsymbol{\kappa}\cdot\mathbf{r}}\varphi_0(\kappa)d^3\kappa$$

$$\tilde{U}(\kappa) = \frac{1}{2\pi^2\kappa^2}, \quad \varphi_0(\kappa) = \frac{\sqrt{8}}{\pi\left(1+\kappa^2\right)^2}$$

Eq. (3) could be transformed to be

$$f_{\downarrow\uparrow,\uparrow\downarrow} = -(2\pi)^2\left\{\int \varphi_0^*(\mathbf{p}_1+\boldsymbol{\kappa})\,\varphi_0(\mathbf{p}_2+\boldsymbol{\kappa})\,\tilde{U}_{12}(\kappa)d^3\kappa + \right.$$
$$\left.\varphi_0(p_2)\int \varphi_0^*(\mathbf{p}_1+\boldsymbol{\kappa})\,\tilde{U}_m(\kappa)d^3\kappa\right\} \tag{4}$$

We have $p_{1,2} \gg 1$ (the necessary condition for the Born approximation), and we can see that $\varphi_0(p)$ for $p \to \infty$ decreases faster than $\tilde{U}(p)$. Therefore, the integration domains where the argument of one of the wavefunctions, $\varphi_0(\tilde{\kappa})$, is of the order of 1 play the dominant role. In both integrals $\kappa \approx |\mathbf{p}_{1,2}| \equiv p$, and we can factor $\tilde{U}(p)$ outside of the integrals, after which they are easily calculated (compare to Problem 4.17):

$$\int \varphi_0^*(\mathbf{p}_1+\boldsymbol{\kappa})\,\varphi_0(\mathbf{p}_2+\boldsymbol{\kappa})\,d^3\kappa = \int \varphi_0^*(\kappa')\,\varphi_0(\mathbf{q}+\boldsymbol{\kappa}')\,d^3\kappa' =$$
$$= \int \varphi_0^*(\kappa')\,\hat{T}_q\varphi_0(\kappa')\,d^3\kappa' = \int e^{-i\mathbf{q}\cdot\mathbf{r}}\,|\psi_0(r)|^2\,dV =$$
$$= \frac{16}{\left(4+q^2\right)^2}, \quad \mathbf{q} = \mathbf{p}_2 - \mathbf{p}_1$$

(the integral has been reduced to the form factor of the hydrogen atom), and

$$\int \varphi_0^*(\mathbf{p}_1+\boldsymbol{\kappa})\,d^3\kappa = (2\pi)^{3/2}\psi_0^*(0) = \sqrt{8}\pi$$

As a result, we obtain the amplitude of the process considered:

$$f_{\downarrow\uparrow,\uparrow\downarrow}(\mathbf{p}_2,\mathbf{p}_1) = -\frac{32}{p^2}\left\{\frac{1}{\left(4+q^2\right)^2} - \frac{1}{2\left(1+p^2\right)^2}\right\}, \quad \mathbf{q} = \mathbf{p}_2 - \mathbf{p}_1 \tag{5}$$

We can see that the region of values $q \lesssim 1$, i.e., of scattering angles $\theta \lesssim 1/p$, plays the dominant role in scattering. The second term in Eq. (5) is negligibly small, so the differential, $d\sigma/d\Omega = |f|^2$, and total scattering cross-sections become equal to

$$\frac{d\sigma}{d\Omega} = \frac{4}{p^4\left(1+p^2\theta^2/4\right)^4}, \quad \theta \lesssim \frac{1}{p}; \quad \sigma = \frac{16\pi}{3p^6} = \frac{16\pi a_B^2}{3\left(ka_B\right)^6} \tag{6}$$

In conclusion here, note the following:

1. The electron scattering cross-section for a hydrogen atom with spin-flip, which is practically inelastic, for large energies is much lower than the elastic scattering cross-section, $\sigma_{el} = 7\pi/3p^2$. See Problem 13.4.

2. The appearance of the small factor, $\sim 1/(pa_B)^2$, in the amplitude (and $\sim 1/(pa_B)^4$ in the cross-section) compared to the case of elastic scattering (no spin flip) has a simple explanation. To "switch" places, the electrons must be scattered into one another under the angle $\approx 180^\circ$ in the center-of-inertia system. The dependence of the Rutherford scattering amplitude on momentum transferred, $f \sim \tilde{U}(q) \sim 1/(pa_B)^2$, gives rise to this smallness (here $q \approx p$; in the case of elastic scattering $qa_B \sim 1$, the value $q_{\min} \sim 1/a_B$ here is due to screening of the Coulomb potential at the distances $\sim a_B$).

3. It is essential that in the process considered, the two particles (two electrons) receive a large momentum change, and that it could be provided by a single interaction. In other reactions with a particle redistribution of the form $a + (bc) \to b + (ac)$, in the case $m_a \neq m_b$, we have $p_a \neq p_b$ and the large change of the momenta of a and b particles requires an additional large momentum transfer to particle c. This leads to the appearance of an additional small factor in the process amplitude [371] $\sim \tilde{U}(q)/q^2$. Such a situation takes place in process (1) for scattering angles that are not too small, when $q \gg 1$, as is seen from Eq. (5). The additional smallness is connected to the fact that the amplitude of the process includes the hydrogen atom wavefunction (or that of the composite system, in the more general case), $\varphi(p)$, that for large momenta ($p \sim q \gg 1$) has an asymptote of the form $\varphi(p) \sim \tilde{U}(p)/p^2 \sim 1/p^4$ (for s-states, compare to Problems 4.17 and 4.18). The factor mentioned has the same order of magnitude as the second-order terms in the T-operator. In this case, when the change of momentum for all particles is large, calculations of the amplitude and cross-section, using first order of perturbation theory, have only qualitative character. A systematic and reliable calculation of the asymptote needs the inclusion of terms of higher order in the T-operator. For processes with large momentum change for all particles in a three-particle system, as, for example, in the conditions of Problem 13.79, we should take into account terms of at least 2nd order in the interaction, $V_{\alpha,\beta}$.

GKKG.13.79

Evaluate the charge-exchange cross-section for the collision of a fast positron with a hydrogen atom in the ground state (i.e., find the cross-section of positronium formation - a hydrogen-like system with an electron and a positron).

Use the Oppenheimer-Brinkman-Kramers approximation (OBK) for the chargeexchange processes, which neglects the mutual interaction of the nuclei involved (in this case, positron with proton); compare with the previous problem.

Solution

The Oppenheimer-Brinkman-Kramers approximation for the charge-exchange process $e_+ + (e_- p) \to (e_+ e_-) + p$ is based on the following expression for the T-operator [372]

$$\hat{T} \approx V_\alpha \approx U_{e^+e^-} = -\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

where $\mathbf{r}_{1,2}$ are the radius vectors of the positron (electron). We will denote the momentum of the incident positron as $\mathbf{p}_1$ (in the rest system of the hydrogen atom, $m_p = \infty$), and the momentum of the positronium as $\mathbf{p}_2$ (with mass $m(e^+e^-) = 2$). From the energy conservation law, it follows that $p_2 = \sqrt{2}p_1$ $\left(E = p_1^2/2 = p_2^2/4\right.$, and we can neglect the binding energy in the hydrogen atom and in the positronium, since $p_{1,2} \gg 1$).

The wavefunctions of the initial (channel α) and final (channel β) states have the form:

$$\psi_\alpha = e^{i\mathbf{p}_1 \cdot \mathbf{r}_1} \psi_{1s}(r_2), \quad \psi_\beta = \exp\left\{\frac{i}{2}\mathbf{p}_2 \cdot (\mathbf{r}_1 + \mathbf{r}_2)\right\} \cdot \frac{1}{\sqrt{8}} \psi_{nlm}\left(\frac{\mathbf{r}_1 - \mathbf{r}_2}{2}\right)$$

Here, $\psi_{nlm}(\mathbf{r})$ is the wavefunction of the hydrogen atom (with mass $m = 1$). Coefficient $1/\sqrt{8}$ and factor $1/2$ in the argument of the wavefunction correspond to the fact that the Bohr radius for positronium is twice that of the hydrogen atom.

The amplitude of the process in the OBK-approximation is described by the expression (after the substitution $\boldsymbol{\rho} = (\mathbf{r}_1 - \mathbf{r}_2)/2$):

$$T_{OBK}(1s \to nlm) = \langle \beta | U_{e^+e^-} | \alpha \rangle = -\sqrt{2} \int \psi_{1s}(r) e^{i(\mathbf{p}_1 - \mathbf{p}_2)\cdot \mathbf{r}} dV \times$$
$$\int \frac{1}{\rho} \psi^*_{nlm}(\boldsymbol{\rho}) e^{-i(\mathbf{p}_2 - 2\mathbf{p}_1)\cdot \boldsymbol{\rho}} d^3\rho \qquad (1)$$

The first integral in this expression is equal to $(2\pi)^{3/2}\varphi_{1s}(q)$ (with $\mathbf{q} = \mathbf{q}_1 - \mathbf{q}_2$), while the second, with the Schrdinger equation taken into account, is

[372] The same results follow also from the choice $T \approx V_\beta \approx U_{e^-p}$. See the previous problem, where we made general statements about processes with a particle redistribution. Let us note that for the charge-exchange

processes, the results of both exact amplitude calculations in the first order of perturbation theory according to $T = V_{\alpha,\beta}$ and in the OBK-approximation have only qualitative character (a reliable calculation necessitates the inclusion of second-order second-order terms).

$$(2\pi)^{3/2}\left(\frac{1}{2}q_1^2 - E_n\right)\boldsymbol{\phi}^*_{nlm}(\mathbf{q}_1), \text{ where } \mathbf{q}_1 = 2\mathbf{p}_1 - \mathbf{p}_2$$

Since $q, q_1 \gg 1$, we can use asymptotes for wavefunctions $\varphi(\mathbf{p})$ in the Coulomb potential, $U = -1/r$ (so $\tilde{U}(p) = -1/2\pi^2 p^2$), for $p \to \infty$. According to Problem 4.18:

$$\varphi_{1s}(p) = \frac{\sqrt{8}}{\pi p^4}, \quad \varphi_{nlm}(\mathbf{p}) = \sqrt{\frac{2}{\pi}}\frac{2(l!)}{p^{l+4}}(-2i)^l \tilde{R}_{nl}(0) Y_{lm}(\mathbf{n}) \tag{2}$$

To obtain this we used a relation for the coordinate Coulomb wavefunctions:

$$\psi_{nlm}(\mathbf{r}) = Y_{lm}(\mathbf{n}) r^l \tilde{R}_{nl}(r), \quad \tilde{R}_{nl}(0) = \frac{2^{l+1}}{(2l+1)! n^{l+2}}\sqrt{\frac{(n+l)!}{(n-l-1)!}}$$

Using these asymptotes, we obtain

$$T_{OBK}(1s \to nlm) = -\frac{16\sqrt{2\pi^3}(\sqrt{2}i)^l \tilde{R}_{nl}(0) l! Y_{lm}(\mathbf{n}_0)}{(3 - 2\sqrt{2}\cos\theta)^{3+l/2} p_1^{6+l}} \tag{3}$$

We have used $\mathbf{n}_0 = (-\mathbf{p}_2 + 2\mathbf{p}_1)/(|\mathbf{p}_2 - 2\mathbf{p}_1|)$, and also that $q_1^2 = 2q^2 = 2(3 - 2\sqrt{2}\cos\theta)p_1^2$, where θ is the angle between vectors $\mathbf{p}_2$ and $\mathbf{p}_1$.

This angular distribution of the emitted positronium, [373] $d\sigma/d\Omega = |T|^2/\sqrt{2}\pi^2$, has several interesting properties. It does not depend on the value of the incident positron's momentum. It is sharply anisotropic (the values of $3 - 2\sqrt{2}\cos\theta$ for angles $\theta = 0$ and π differ by a factor of 35). The polarization state of the positronium created is characterized by a definite projection of its angular momentum onto the direction of vector $\mathbf{n}_0, m_n = 0$, since $Y_{lm}(\theta = 0) = \sqrt{(2l+1)/4\pi}\delta_{m,0}$. For the total chargeexchange cross-section, after summing over the values of the projection of the angular momentum, m, of the positronium created, we obtain

$$\sigma_{OBK}(1s \to nl) = 64\pi a_B^2 \frac{2^l (2l+1)(l!)^2 \tilde{R}^2_{nl}(0)}{(l+5)(3-2\sqrt{2})^{5+l}} \frac{1}{V^{12+2l}} \tag{4}$$

where $V = p_1 a_B/\hbar$ is the relative velocity of the colliding positron and hydrogen atom in atomic units. In particular, we can write the charge-exchange cross-section for the ns-states of the positronium as

$$\sigma_{OBK}(1s \to ns) = \frac{\pi a_B^2}{n^3}\left(\frac{2.89}{V}\right)^{12} \tag{5}$$

Pay attention to the pronounced energy-dependence of the charge-exchange cross-section, $\sigma \propto p^{-12-2l}$ (compare with the result of the previous problem and with the case of elastic scattering; see Problem 13.4). It is explained by the fact that all particles involved experience a large change of momentum. In connection with this, we should note that the charge-exchange cross-section for collisions of fast heavy particles $m \gg m_e$ with a hydrogen atom have a similar energy-dependence. For $m \gg m_e$, the

charge-exchange cross-section does not depend on the mass of the incident particle (for example, proton, muon, etc.). In particular, the charge-exchange cross-section in the ns-state is
$$

$$\sigma_{OBK}(1s \to ns) = \pi a_B^2 \frac{2^{18} Z^5}{5 n^3 V^{12}} \approx \frac{\pi a_B^2}{n^3} Z^5 \left(\frac{2.47}{V}\right)^{12} \tag{6}$$

$$
where Z is the particle charge. From comparison of Eqs. (5) and (6), we see that the charge-exchange cross-section for the collision of the positron and hydrogen atom is ≈ 7 times larger than for the collision with a proton (for the same velocities).

GKKG.13.80

In the Born approximation, express the amplitude of the process $A_i + B_i \to A_f + B_f$ for the collision of fast composite particles A and B, interacting electrostatically, through electric form-factors [374]

$$eF^{A(B)}_{if}(\mathbf{q}) = \left\langle \psi_{A(B)f} \right| \sum_a e_a \exp\{-i\mathbf{q}\cdot\mathbf{r}_a\} \left| \psi_{A(B)i} \right\rangle$$

[0] [373] See Problem 13.78 for amplitude normalization. In this problem, $\mu_1 = 1, \mu_2 = 1, p_2 \approx \sqrt{2}p_1$.

for transitions $i \to f$.
Consider the behavior of the form-factor for $q \to 0$, depending on the quantum numbers of the initial and final states.

Calculate the form-factors for transitions $1s \to 1s, 1s \to 2s, 1s \to 2pm$ in the hydrogen atom. Consider their behavior as $q \to \infty$.

Find the collision cross-section for the following processes:

1. $H(1s) + H(1s) \to H(1s) + H(1s)$, elastic scattering of hydrogen atoms from one another;

2. the collision of a charged, structureless particle (electron, muon, proton, etc., but not an ion) with a hydrogen atom in the ground state, accompanied by the excitation of a) $2s$ state in the atom; b) $2p$ states in the atom.

Solution

Let us denote the radius vectors of the $A(B)$ particles' centers of mass by $\mathbf{R}_{A(B)}$, their masses by $m_{A(B)}$, and the momenta of their relative motion by $\mathbf{p}_{1,2}$ (1) before and (2) after the collision. The wavefunctions of the initial and final states have the form: [375]

[374] Let us emphasize that $\mathbf{r}_a$ is the radius vector of the a th charged particle in the composite system $A(B)$ with respect to the system's center-of-mass.

[375] Wavefunctions $\psi_{A(B)}$ of the composite particles describe the states of the particles in the composite system, with respect to its center-of-mass.

$$\psi_i = \exp\left\{\frac{i}{\hbar}\mathbf{p}_1 \cdot \mathbf{R}\right\} \psi_{Ai}\left\{x'_a\right\} \psi_{Bi}\left\{r'_B\right\}, \quad \mathbf{R} = \mathbf{R}_A - \mathbf{R}_B,$$
$$\psi_f = \exp\left\{\frac{i}{\hbar}\mathbf{p}_2 \cdot \mathbf{R}\right\} \psi_{Af}\left\{x'_a\right\} \psi_{Bf}\left\{r'_B\right\}, \quad \hbar\mathbf{q} = \mathbf{p}_2 - \mathbf{p}_1, \tag{1}$$

The amplitude of the process considered in the Born approximation is described by the expression (compare to Problems 13.77 and 13.78):

$$f_{if} = -\frac{\mu}{2\pi\hbar^2} T_{if} = -\frac{\mu}{2\pi\hbar^2} \left\langle \psi_f \right| \sum_{a,b} \frac{e_a e_b}{|\mathbf{x}_a - \mathbf{r}_b|} \left| \psi_i \right\rangle, \quad \frac{d\sigma}{d\Omega} = |f|^2 \tag{2}$$

We use $\mu = m_A m_B / (m_A + m_B)$, the reduced mass of particles A and B. The integration in matrix element (2) is performed both over independent "inner" coordinates $\mathbf{x}'_a$, $\mathbf{r}'_b$ (in the case of atoms, these are the coordinates of all electrons), and over the radius vector, $\mathbf{R}$, of the relative motion. Writing here $\mathbf{x}_a = \mathbf{R}_A + \mathbf{x}'_a$ and $\mathbf{r}_b = \mathbf{R}_B + \mathbf{r}'_b$, using the form of the wavefunctions (1), and using the Fourier transform of the Coulomb potential

$$\frac{1}{|\mathbf{x}_a - \mathbf{r}_b|} = \frac{1}{2\pi^2} \int \exp\left\{i\boldsymbol{\kappa}\left(\mathbf{x}_a - \mathbf{r}_b\right)\right\} \frac{d^3\kappa}{\kappa^2}$$

we obtain

$$T_{if} = \frac{4\pi e^2}{q^2} F_{if}^A(-\mathbf{q}) F_{if}^B(\mathbf{q}) \tag{3}$$

Here

$$eF_{if}^{A(B)}(\mathbf{q}) = \left\langle \psi_{A(B)f} \right| \sum_a e_a \exp\left\{-i\mathbf{q} \cdot \mathbf{r}'_a\right\} \left| \psi_{A(B)i} \right\rangle \tag{4}$$

are the electric form-factors for the corresponding transitions in the composite particles $A(B)$. We can associate the Feynman diagram in Fig. 13.8 with the amplitude, Eq. (3).

It illustrates an important property of the amplitude: it is factorized in terms of the particles, A and B, that take part in the process. In this figure, the wavy line between the vertices corresponds to $4\pi/q^2$, while the form-factors $eF_{if}^{A(B)}(\mp\mathbf{q})$ correspond to the vertices (note that the changes in the momenta of particles A and B differ by a sign).

Let us note some properties of the form-factors:

1. For point (structureless) particles, $F(q) = Z = \text{const}$, where Ze is particle charge.

2. For $q \to 0$, expanding $\exp\{-i\mathbf{q}\cdot\mathbf{r}\}$ in Eq. (4) for $F(\mathbf{q})$ into a series reveals that for a system with charge Ze different from zero, only the elastic (without a change of composite particle's state) form-factor is different from zero, and is equal to $F_{nn}(0) = Z$. In all other cases $F_{if}(0) = 0$ (for a charged particle, due to wavefunction orthogonality). The character of how exactly the form-factor vanishes in the limit $q \to 0$ depends on the quantum numbers, angular momenta, and parity

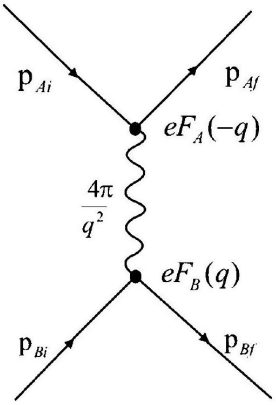


Fig. 13.8

of the initial and final states. The slowest decrease in the form factor is for the dipole transitions: $eF_{if} \approx -i\langle f|\hat{\mathbf{d}}|i\rangle q \propto \mathbf{q}$. For transitions with unchanging values of the angular momentum and parity (for example, for S-states), $F_{if} \propto q^2$. With an increase in the difference between the angular momenta of the initial and final states, the form-factor goes to zero for $q \to 0$ more abruptly.

3) For $q \to \infty$ the form-factor of any composite system vanishes. [376] The power law of this decrease depends strongly on the number of particles in the system and on the specific interaction. From physical considerations, it is evident that the faster $\bar{U}(q)$ decreases and the larger the particle number in the compound system, the faster the form-factor decreases. Compare to Problem 13.84.

For transitions of the hydrogen atom, the form-factors

$$F_{1s\to nlm}(q) = \int \psi^*_{nlm}(\mathbf{r})\left(1 - e^{-i\mathbf{q}\cdot\mathbf{r}}\right)\psi_{1s}(r)dV$$

are easy to calculate. Taking into account the form of the wavefunctions (see Eq. (IV.4)), we can obtain

$$F_{1s\to 1s} = 1 - F_{at}(q) = \frac{8q^2 + q^4}{(4+q^2)^2}, \quad F_{1s\to 2s} = -\frac{4\sqrt{2}q^2}{(9/4+q^2)^3} \tag{5}$$

[376] For an atom in the approximation of an infinite nuclear mass, for $q \to \infty$ the elastic form-factor is $F_{el} = Z$ (it is determined by the contribution from a point-like nucleus).

For the $2p$-states, it is convenient to write the angular part of the wavefunction in the form $\sqrt{3/4\pi}\varepsilon(m)\cdot\mathbf{n}$, where $|\varepsilon(m)|^2 = 1$ (compare Problems 3.41 and 3.42), after which we obtain

$$F_{1s\to 2pm} = -\frac{\varepsilon^*(m)}{4\sqrt{2\pi}}\frac{i\partial}{\partial\mathbf{p}}\int \exp\left\{-\frac{3r}{2} - i\mathbf{q}\cdot\mathbf{r}\right\}dV = \\ = 6\sqrt{2}i\frac{\varepsilon^*(m)\mathbf{q}}{(9/4+q^2)^3} \tag{6}$$

This form-factor is different from zero only for the states with projection of the angular momentum on the direction of the vector $\mathbf{q}$ equal to zero.

For calculating the scattering cross-sections, we first note that

$$q^2 = p_1^2 + p_2^2 - 2p_1p_2\cos\theta, \quad p_2 = \sqrt{p_1^2 - 2\mu(\varepsilon_1 - \varepsilon_2)} \approx \\ \approx p_1 - \frac{\mu(\varepsilon_1 - \varepsilon_2)}{p_1}$$

where $\varepsilon_{1,2} > 0$ are the binding energies of the system before and after the collision. So $d\Omega$ could be replaced by $\pi dq^2/p_1^2$, with the integration over q^2 within limits 0 and ∞ (due to the fast convergence in the upper limit, $q^2_{\max} \approx 4p_1^2$). We cannot always replace the lower integration limit

$$q^2_{\min} = (\mathbf{p}_1 - \mathbf{p}_2)^2 \approx \left(\frac{\mu(\varepsilon_1 - \varepsilon_2)}{p_1}\right)^2$$

by 0, because of a divergence that may appear. This complication however only arises for the inelastic collisions where one of the colliding particles has charge different from zero and its state during the collision

process does not change, so that for it, $F(0) = Z \neq 0$, and for the other particle, the transition is of dipole type. Thus, $eF_{if} \approx -i\mathbf{d}_{if}\mathbf{q}$ for $q \to 0$.

Elementary integration gives the following results:

$$1)\ \sigma(1s1s \to 1s1s) = \frac{4\pi}{V^2}\int\limits_0^\infty F^4_{1s\to 1s}(q)dq^2 = \frac{33\pi}{35V^2} \tag{7}$$

$$2)\ \sigma(1s \to 2s) = \frac{4\pi Z^2}{V^2}\int\limits_0^\infty F^2_{1s\to 2s}(q)dq^2 = \frac{2^{17}\pi Z^2}{5\cdot 3^{10}V^2} \approx 0.444\frac{\pi Z^2}{V^2} \tag{8}$$

where $V = p_1/\mu$ is the relative velocity of the colliding particles, and Ze is the charge of the particle colliding with the hydrogen atom.

Now we calculate the total cross-section for collisions with transitions $1s \to 2p$, by summing over the transitions $1s \to 2pm$:

$$\sigma(1s \to 2p) = 288\pi\left(\frac{Z}{V}\right)^2\left(-\frac{1}{5!}\frac{\partial^5}{\partial a^5}\int\limits_{q^2_{min}}^\infty \frac{dx}{x(a+x)}\right) = \tag{9}$$

$$288\pi\left(\frac{Z}{V}\right)^2\frac{1}{5!}\left[-\frac{\partial^5}{\partial a^5}\left(\frac{1}{a}\ln\frac{a}{q^2_{min}}\right)\right] = \frac{2^{17}\pi Z^2}{3^{10}V^2}\left[\ln\left(16V^2\right) - \frac{137}{60}\right]$$

where $x = q^2, a = 9/4, q^2_{\min} = \left(\varepsilon_{2p} - \varepsilon_{1s}\right)^2/V^2 = 9/64V^2$. Finally,

$$\sigma(1s \to n = 2) = \frac{2^{18}\pi Z^2}{3^{10}V^2}\left(\ln 4V - \frac{25}{24}\right) \approx 4.44\frac{\pi Z^2}{V^2}\left(\ln 4V - \frac{25}{24}\right) \tag{10}$$

is the total cross-section of exciting the states of the hydrogen atom with the principal quantum number $n = 2$ by collision with a charged particle.

Б-2.12.7 Рассеяние нейтрона на молекуле водорода (???)

Записать выражение для эффективного псевдопотенциала, описывающего рассеяние медленного нейтрона на молекуле водорода H_2.

Solution.

GKKG.13.81

Consider the collision between a fast charged particle and a two-atom molecule in its ground state with the dipole moment, d_0. The electron term of the molecule is $^1\Sigma$. Estimate the cross-sections of collisions, which involve excitation of the rotational and oscillation molecular levels. Compare to the case of the collision with an atom (see the previous problem).

Solution

As in the previous problem, the collision cross-section is connected to the electric form-factor of the molecule,

$$eF_{0\to vKM}(\mathbf{q}) = \langle n, \Lambda = 0, vKM|\sum_a e_a e^{i\mathbf{q}\cdot\mathbf{r}_a}|n, 0\rangle \tag{1}$$

In the initial state, the quantum numbers are $\Lambda = v = K = M = 0$, while n characterizes the state of molecular electrons. The wavefunctions of the molecululars states with $\Lambda = 0$, as are in matrix element (1), have the form:

$$\psi_n\Lambda = 0vKM = \psi^{el}_{n\Lambda=0}\left(\xi_a, \mathbf{R}\right)\psi^{osc}_v\left(\mathbf{R} - \mathbf{R}_0\right)Y_{KM}(\mathbf{n}) \tag{2}$$

Here ξ_a are the electron variables (coordinate and spin); $\mathbf{R} = R\mathbf{n} = \mathbf{R}_1 - \mathbf{R}_2$ is the radius vector from one nucleus to the other; the masses are $M_{1,2}$; and the radius vectors in the molecule's center-of-mass system: $\mathbf{R}_1 = M_2\mathbf{R}/\left(M_1 + M_2\right)$ and $\mathbf{R}_2 = -M_1\mathbf{R}/\left(M_1 + M_2\right)$. Summation in Eq. (1) is performed over both the molecular electrons ($\mathbf{r}_a$ denotes the radius vectors relative to the molecular center of mass), and the nuclei, whose contribution is $Z_1e^{-i\mathbf{q}\cdot\mathbf{R}_1} + Z_2e^{-i\mathbf{q}\cdot\mathbf{R}_2}$.

We write the cross-section for the collision between the charged particle and the molecule,

$$\frac{d\sigma_{0\to vKM}}{d\Omega} = \left(\frac{2\mu Ze^2}{\hbar^2 q^2}\right)^2 |F_{0\to vKM}(\mathbf{q})|^2 \tag{3}$$

where Ze is particle charge, and μ is its and the molecule's reduced mass. We note that the easiest way to obtain these cross-sections is to neglect the change in the state of the valence electron states in the molecular formation. In this approximation, the wavefunction of the electron term of the molecule is

$$\psi^{\text{elec}}_{n\Lambda=0} \approx \psi_1(\mathbf{r}_a - \mathbf{R}_1)\,\psi_2(\mathbf{r}_b - \mathbf{R}_2)$$

where $\psi_{1,2}(\mathbf{r}_{a,b})$ is the wavefunction for the electron bound to a single atom of the molecule, and for its form-factor, we obtain

$$F_{0\to\nu KM} \approx \langle \nu KM| \left(e^{-iR_1\mathbf{q}\cdot\mathbf{n}}F_1(q) + e^{iR_2\mathbf{q}\cdot\mathbf{n}}F_2(q)\right)|0\rangle \tag{4}$$

where $F_{1,2}(q)$ are the form-factors of the atoms in the molecule (which also include contributions of the corresponding nuclei). Note that for $q = 0$, the form-factor of the molecule, as of any neutral system, is equal to zero (see a discussion of form-factors in the previous problem).

Due to the smallness of amplitude of nuclear oscillations, we can replace $\mathbf{R}_{1,2}$ by their equilibrium positions. Then, due to wavefunction orthogonality, only the formfactors for transitions with $v = 0$ (i.e., without a change of the molecular oscillation state) are non-zero. For such transitions, we can calculate the differential cross-section, Eq. (3), by summing over the values of the quantum numbers K and M of the molecule's final states. Using approximation (4) and the completeness condition for the spherical functions, according to which

$$\sum_{KM} |\langle KM|\hat{A}|0\rangle|^2 = \sum_{KM}\langle 0|\hat{A}^+|KM\rangle\langle KM|\hat{A}|0\rangle = \langle 0|\hat{A}^+\hat{A}|0\rangle$$

we calculate the differential cross-section:

$$\sum_{KM}\frac{d\sigma_{0\to 0KM}}{d\Omega} = \left(\frac{2\mu Ze^2}{\hbar^2 q^2}\right)^2 \left\langle 0\|F_1(q) + F_2(q)e^{i\mathbf{q}\cdot\mathbf{R}_0}\right|^2|0\right\rangle$$

Compare to Problem 13.7.

Collision cross-sections that do not excite molecular oscillations obey the same rules as the case of a charged particle colliding with an atom (compare to the previous problem). In particular, for collisions that excite a rotational level with the angular momentum $K \neq 1$, the cross-section is

$$\sigma_{0\to 0KM} = \pi a_B^2 Z^2 A_{KM}\left(\frac{V_{at}}{V}\right)^2, \quad K \neq 1 \tag{5}$$

where V is the relative velocity of the colliding particles, and $A_{KM} \sim 1$ for the most important transitions.

For collisions that excite a rotational level with $K = 1$, connected to the ground level by a dipole transition, [377] for $q \to 0$ we have (compare to the previous problem):

$$\frac{d\sigma(0\to 0M)}{dq^2} = \frac{4\pi Z^2 e^2 d_0^2}{3\hbar^2 q^4 V^2}|\varepsilon(M)\mathbf{q}|^2 \tag{6}$$

$\varepsilon(M)$ is the polarization vector that determines a molecular rotational state with $K = 1$, and is connected to the spherical functions by the relation $Y_{1M} = \sqrt{3/4\pi}\varepsilon(M)\mathbf{n}$, where $|\varepsilon|^2 = 1$. Eq. (6) follows from expressions (1) and (3) if we take into account that: 1) for $q \to 0$, the sum in (1) becomes $-i\mathbf{q}\cdot\mathbf{d}$, where $\mathbf{d}$ is the operator of the molecular dipole moment; 2) averaging $\mathbf{d}$ over the electron states of the molecule with $\Lambda = 0$ gives $d(R)\mathbf{n}$; 3) after averaging over the oscillation states with $v = 0$, we can replace $d(R)$ by $d(R_0) \equiv d_0$ due to the smallness of the nuclear oscillation amplitudes (compare to Problem 11.25). The summation in Eq. (6) over M gives $\sum|\varepsilon(M)\mathbf{q}|^2 = q^2$, and the following integration over q^2 with the lower limit of integration (to cut off a divergence) being

$$q^2_{\min} = \left[\frac{\hbar}{\tilde{\mu}R_0^2 V}\right]^2$$

($\tilde{\mu}$ is the reduced mass of the molecular nuclei) allows us to obtain the cross-section of transitions to states with $K = 1$ to logarithmic accuracy: [378]

$$\sigma(0\to v = 0, K = 1) \approx \frac{8\pi Z^2 e^2 d_0^2}{3\hbar^2 q^4 V^2}\ln\frac{\tilde{\mu}}{m_e V_{at}} \tag{7}$$

Let us properties of the collision processes, accompanied by excitation of the molecular oscillation levels. As was mentioned before, replacement of R by is equilibrium value R_0 due to the weak nuclear oscillations is valid only for transitions that do not excite oscillations. For states with $v \neq 0$, in this approximation, the form-factor goes to zero due to wavefunction orthogonality. So for transitions with $v \neq 0$, it is necessary to perform expansion over the small parameter $\Delta R/R_0$, where $\Delta R = R - R_0$ is of the order of the nuclear oscillation

amplitudes. For the linear expansion term, which corresponds to transitions with $\Delta v = 1$, in expression (1) for $v = 1$, as opposed to $v = 0$, a small factor appears, on the order of (see Problems 11.3 and 11.25)

$$\langle v = 1|\frac{R - R_0}{R_0}|v = 0\rangle = \frac{a_{osc}}{\sqrt{2}R_0} \sim \left(\frac{m_e}{\tilde{\mu}}\right)^{1/4}$$

[377] For this transition, approximation (4) for $q \to 0$ is not valid; the dipole moment of the molecule is determined by its valence electrons.

[378] Here as usual, for the upper integration limit we choose the value $q^2_{\max} \sim a_B^{-2}$. We should note that although the argument of the logarithm in Eq. (7) is much larger than in the case of a dipole transition in an atom, due to the small rotational energy, nevertheless the accuracy of Eq. (7) does not increase because of it. Usually, the dipole moment of the molecule, d_0, is much smaller than the value ea_B

This leads to much lower, $\sim (\tilde{\mu}/m_e)^{1/2}$, cross-sections of the transitions with $v = 1$. With an increase of the value v, it is necessary to consider higher orders in $\Delta R/R_0$, which leads to a sharper, $\sim (\mu/m_e)^{v/2}$, suppression of the cross-section for the corresponding molecular transitions.

GKKG.13.82

Find the cross-section of a fast charged particle colliding with a hydrogen atom in a metastable $2s$-state, accompanied by its transition into a $2p$-state.

Comment: In this problem it is necessary to take into account the relativistic splitting of the s - and p-levels (see Problem 11.62).

Solution

For collisions of a charged particle and an atom accompanied by an atomic dipole transition, the region with small values of q^2 plays the dominant role. The cross-section of the collision with transition from the s - to the p-state of the atom to logarithmic accuracy is described by the expression (compare to Problem 13.80):

$$\sigma_{s\to p} = \frac{4\pi Z^2 e^2}{\hbar^2 V^2} \left|\langle l = 1, m = 0|d_z|\, 0\right\rangle|^2 \ln \frac{1}{q^2_{\min} a_B^2} \tag{1}$$

where Ze is the charge of the incident particle and V is the relative velocity of the colliding particles. For a transition $2s \to 2p$ in the hydrogen atom, the matrix element [379] $\langle 1, 0|d_z|0\rangle = 3ea_B$ was calculated in Problem 11.33, in connection with the Stark effect for the states with $n = 2$.

If we neglect relativistic corrections, the states $2s$ and $2p$ of the hydrogen atom are degenerate; here $q^2_{\min} = 0$ and the cross-section, Eq. (1), diverges. Splittings, Δ, of the levels $2s_{1/2}, 2p_{1/2}$ and $2p_{3/2}$, which determine the values of $q^2_{\min} = (\Delta/\hbar V)^2$, were discussed in Problem 11.62. Since here, transitions into the atomic states $2p_{1/2}$ and $2p_{3/2}$ must be considered separately, it is necessary to add the additional factors, equal 1/3 and 2/3, for the $p_{1/2}$- and $p_{3/2}$-states, in Eq. (1). These factors, the squares of the corresponding Clebsch-Gordan coefficients (see, for example, Problem 5.18), reflect the contribution of p-states with $l_z = 0$ to the states [380] $p_{1/2}$ and $p_{3/2}$. If we take into account these facts, we find

$$\sigma(2s \to 2p) = 72\pi a_B^2 \left(\frac{Ze^2}{\hbar V}\right)^2 \ln \frac{\hbar V}{a_B \Delta_0^{1/3} \Delta_1^{2/3}} \tag{2}$$

where $\Delta_0 = E\left(2s_{1/2}\right) - E\left(2p_{1/2}\right)$ and $\Delta_1 = E\left(2p_{3/2}\right) - E\left(2s_{1/2}\right)$, with the numerical value $\Delta_0^{1/3}\Delta_1^{1/3} \approx 8 \cdot 10^{-7}$ (in atomic units).

[379] We emphasize that Eq. (1) describes the cross-section, summed over the projections of the angular momentum of the p-state. Although in Eq. (1) there is a state with $l_z = 0$, we should remember that the choice of a quantization axis z, along the vector $\mathbf{q}$, depends on the scattering angle.

[380] If we take into account relativistic corrections, l_z is not a constant of the motion.

As is seen from Eq. (2), the cross-section $\sigma \gg (V_{at}/V)^2 \sigma_0$, where $\sigma_0 = \pi\overline{r^2} = 40\pi a_B^2$, characterizes the transverse size of the hydrogen atom in states [381] with $n = 2$. This means that in this problem, large impact parameters ($\gg a_B$) are essential. Effective interaction at such distances is $Ze\mathbf{d} \cdot \mathbf{r}/r^3 \sim Zed/r^2$. The applicability condition of perturbation theory (see Eq. (XIII.7)) for such a potential is fulfilled for the distances $r \gg Zed/\hbar V$. Even for values $V \approx 1$, this condition holds true, which proves the applicability of Eq. (2) for such collision velocities.

In conclusion, note that the large value of the transition cross-section, (2), implies that the lifetime of the metastable $2s$-state in a gas could decrease sharply due to collisions (for an isolated hydrogen atom, $\tau(2s) = 1/8$ s; while in the presence of transitions in the $2p$-state, the atom "flashes up" within $\sim 10^{-9}$ s).

GKKG.13.83

Calculate (with logarithmic accuracy) the cross-section of fast deuteron fission in the Coulomb field of a nucleus with charge Ze (for simplicity, consider the nucleus to be point-like and infinitely heavy). Choose the deuteron wavefunction as in the case of a zero-range potential (see 12.1), which is reasonable because of the smallness of the proton-neutron binding energy.

Solution

The differential cross-section of deuteron fission is described by the expression:

$$d\sigma_{fis} = \frac{4Z^2e^4m_d^2}{\hbar^2q^4}\left|\langle \mathbf{p},-|e^{-i\mathbf{q}\cdot\mathbf{r}_p}|\,0\right\rangle|^2\,d^3k d\Omega_f \tag{1}$$

Here, $\hbar\mathbf{q} = \mathbf{P}_f - \mathbf{P}_i, \mathbf{P}_i = m_d\mathbf{V}$ is the deuteron momentum, $\mathbf{P}_f$ is the nucleon's total momentum after the collision, $d\Omega_f$ is the infinitesimal solid angle (which contains vector $\mathbf{P}_f$ direction), and $m, m_d = 2m$ are the nucleon and deuteron masses. The Matrix element

$$F_{0\to\mathbf{p}} = \langle \mathbf{p},-|\exp\{-i\mathbf{q}\cdot\mathbf{r}_p\}|0\rangle$$

could be considered as an inelastic form-factor for transitions into the continuum (compare to Problem 13.80). For the wavefunction of the initial state, we write (see Problems 4.10 and 12.1):

$$\psi_0(r) = \sqrt{\frac{\kappa}{2\pi}}\frac{1}{r}e^{-\kappa r}, \quad \varepsilon_0 = \frac{\hbar^2\kappa^2}{m}$$

where ε_0 is the deuteron binding energy, and $\mathbf{r}_p = \mathbf{r}/2$. For the wavefunctions of the final states, we should choose [382] the wavefunction $\psi^-_{\mathbf{k}}(r)$, that has an asymptote in the form of "a plane wave + a converging wave;" they are normalized to $\delta(\mathbf{k}-\mathbf{k}')$.

[381] For the ns-states of the hydrogen atom, $\overline{r^2} = \frac{1}{2}n^2\left(5n^2+1\right)$.

[382] For an alternative convenient choice of final state wavefunctions, see Problem 11.63.

The dominant input into the fission cross-section comes from small q^2, where transitions to states of the two-nucleon system are important, connected to the deuteron's dipole transition, since for them $d\sigma \propto dq^2/q^2$ (compare to Problem 13.80). For such q, we have

$$\langle \mathbf{p},-|\exp\{-i\mathbf{q}\cdot\mathbf{r}_p\}|0\rangle \approx \langle \mathbf{p},-|\left(-i\mathbf{q}\cdot\mathbf{r}_p\right)|0\rangle \tag{2}$$

and in the last expression we can replace the wavefunction $\psi^-_{\mathbf{k}}$by the plane wave $\psi_{\mathbf{k}} = (2\pi)^{-3/2}e^{i\mathbf{k}\cdot\mathbf{r}}$. This is connected to the fact that in a zero-range potential, wavefunctions $\psi^-_{\mathbf{k}}$and $\psi_{\mathbf{k}}$ differ from one another in s-wave only, which does not contribute to the dipole moment, Eq. (2). A calculation of the corresponding matrix element gives

$$\frac{\sqrt{\kappa}\mathbf{q}}{8\pi^2}\frac{\partial}{\partial\mathbf{k}}\int\frac{1}{r}e^{-\kappa r-i\mathbf{k}\cdot\mathbf{r}}d^3r = \frac{\sqrt{\kappa}\mathbf{q}}{2\pi}\frac{\partial}{\partial\mathbf{k}}\frac{1}{k^2+\kappa^2} = -\frac{\sqrt{\kappa}\mathbf{q}\cdot\mathbf{k}}{\pi\left(k^2+\kappa^2\right)^2} \tag{3}$$

The angular dependence $\propto(\mathbf{q}\cdot\mathbf{k})$ of the vector $\mathbf{k}$ reflects the fact that for a dipole transition, the angular momentum of the nucleon pair in the final state is $l = 1$.

To obtain the differential cross-section, we substitute Eq. (3) in Eq. (1) and perform the integration over the directions of the vector $\mathbf{k}$, using the relations

$$d^3k = k^2dkd\Omega, \quad \int(\mathbf{q}\cdot\mathbf{k})^2d\Omega = \frac{4\pi}{3}q^2k^2$$

After this, $d\Omega_f$ in Eq. (1) could be replaced by $\pi\hbar^2dq^2/P_i^2$. Then the value of P_f that follows from the energy conservation law,

$$\frac{1}{2m_d}P_i^2 - \varepsilon_0 = \frac{1}{2m_d}P_f^2 + \varepsilon$$

where $\varepsilon = \hbar^2k^2/m$ is the energy of the nucleon pair's relative motion after the collision, determines

$$\hbar^2q^2_{\min} = (P_f - P_i)^2 \approx \frac{1}{V^2}(\varepsilon+\varepsilon_0)^2$$

Integrating over q^2 within the limits $q^2_{\min}$ and [383] $q^2_{\max} \approx \kappa^2$, we find

$$d\sigma_{fis} = \frac{8\left(Ze^2\right)^2\left(\varepsilon_0\varepsilon^3\right)^{1/2}}{3m\left(\varepsilon+\varepsilon_0\right)^4V^2}\ln\frac{\hbar^2\kappa^2V^2}{\left(\varepsilon+\varepsilon_0\right)^2}d\varepsilon \tag{4}$$

As is seen, the characteristic value of energy is $\varepsilon \sim \varepsilon_0$. The integration of Eq. (4) over ε gives the total cross-section of deuteron electro-fission. With logarithmic accuracy, we can neglect the dependence on ε under the logarithm and obtain (making the substitution $x = \sqrt{\varepsilon}$; see App.1.5)

[383] Note that for larger values of q it is necessary to take into account the finiteness of nucleon size, whose form-factor decreases fast for $q > 1/R$. Since $q^2_{\max}$ in the final result is inside a logarithm, its detailed value is not so important.

$$\sigma_{fis}(E) \approx \frac{\pi \left(Ze^2\right)^2}{6\varepsilon_0 E} \ln \frac{E}{\varepsilon_0} \tag{5}$$

where $E = m_d V^2/2$ is the deuteron energy.
According to Eq. (5), the value of the cross-section for $E = 200\text{MeV}, \varepsilon_0 = 2.2$ MeV is $\sigma_{\text{fis}} = 1.1 \cdot 10^{-28} Z^2$ cm^2. For all nuclei except for perhaps the heaviest, this quantity is much lower than their geometric size, which shows that the dominant role in the process of deuteron fission is nuclear interaction.

We also note a quasi-classical estimation of the fast deuteron fission cross-section accompanied by the escape of one of the nucleons, a proton or a neutron, for a collision with a nucleus with radius R. Considering the potential to be a hard sphere of radius R:

$$\sigma \sim 2\pi R \Delta R, \quad \Delta R \sim R_d \sim \frac{1}{\kappa} \tag{6}$$

This area is that of a ring with radius R and width of the order of the deuteron size.
In conclusion, we note that each escaping nucleon takes away the energy $E_N \approx E/2$ and moves in the direction of the falling beam with the angle of dispersion $\Delta\theta \sim (\varepsilon_0/E)^{1/2}$ (the transverse component of the nucleon momentum $p_\perp \sim \sqrt{m\varepsilon_0}$ is determined by the binding energy of the deuteron).

GKKG.13.84

Find the asymptotic behavior of the electric form-factor of a two-particle system as $q \to \infty$. It is assumed that the Fourier component of the interaction potential, $\tilde{U}(q)$, that is responsible for the formation of the composite system, has a power-law decay at $q \to \infty : \tilde{U}(q) \propto q^{-n}$ with $n > 1$. Compare to Problem 4.18. Consider applications of the results obtained to the hydrogen atom.

Solution

The electric form-factor for the transition between states ψ_1 and ψ_2 of a twoparticle composite system is described by the following expression (see, for example, Problem 13.80):

$$eF_{1\to 2}(\mathbf{q}) = \langle n_2 l_2 l_{2z}| \, e_1 e^{-i\mathbf{q}\cdot\mathbf{r}_1} + e_2 e^{-i\mathbf{q}\cdot\mathbf{r}_2} \, |n_1 l_1 l_{1z}\rangle \tag{1}$$

where $e_{1,2}$ and $m_{1,2}$ are the charges and masses of the particles, $\hbar\mathbf{q}$ is the momentum transferred between systems, and $\mathbf{r}_{1,2}$ are their radius vectors in the center-of-inertia system. Here,

$$\mathbf{r}_1 = \frac{m_2}{m_1 + m_2}\mathbf{r}, \quad \mathbf{r}_2 = -\frac{m_1}{m_1 + m_2}\mathbf{r}, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$$

Eq. (1) includes two integrals:

$$I\left(\mathbf{q}_{1,2}\right) = \int \psi^*_{n_2 l_2 l_{2z}}(\mathbf{r}) \exp\left\{-i\mathbf{q}_{1,2}\mathbf{r}\right\} \psi_{n_1 l_1 l_{1z}}(\mathbf{r}) d^3 r \tag{2}$$

where $\mathbf{q}_{1,2} = \pm m_{2,1}\mathbf{q}/\left(m_1 + m_2\right)$. The asymptotes of these integrals for $q \to \infty$ are determined by the singular terms of the radial wavefunctions in $\psi_{1,2}$ (see Problem 4.18). Let us write

$$\psi_{nll_z}(\mathbf{r}) = \varepsilon_{i\ldots n}\left(l, l_z\right) x_i \ldots x_n \left\{\tilde{R}_{reg}(r) + \tilde{R}_{sin}(r)\right\}$$

where $\tilde{R}_{reg}(r)$ and $\tilde{R}_{sin}(r)$ are the regular and singular parts of the radial function. Remember that the regular part could be expanded into a series over even, $\left(r^2\right)^s$, powers of the variable r, and $\tilde{R}_{reg}(0) \neq 0$, while $\tilde{R}_{\text{sin}}\left(0\right) = 0$. To obtain the asymptote of integral (2), take one of the radial functions at $r = 0$, and keep the singular part of the other, so that

$$\begin{aligned} & I(\mathbf{q})_{q} \to \infty \\ & \approx \varepsilon^*_{i\ldots n}(2)\varepsilon_{s\ldots l}(1) i\frac{\partial}{\partial q_i} \ldots i\frac{\partial}{\partial q_n} i\frac{\partial}{\partial q_s} \ldots i\frac{\partial}{\partial q_l} \times \\ & \times \left\{\tilde{R}_{2reg}(0) \int e^{-i\mathbf{q}\cdot\mathbf{r}} \tilde{R}_{1\,\text{sin}}(r) d^3 r + \tilde{R}_1(0) \int e^{-i\mathbf{q}\cdot\mathbf{r}} \tilde{R}_2 \sin(r) d^3 r\right\} \end{aligned} \tag{3}$$

The singular part for both radial functions is very small for $r \to 0$, and does not effect the leading asymptotic term of the expansion $I(q)$ for $q \to \infty$. The integrals here are connected to the asymptotes of wavefunctions in the momentum representation. According to Problem 4.18, we have:

$$\frac{\hbar^2 q^2}{2\mu}\hat{D}\int e^{-i\mathbf{q}\cdot\mathbf{r}}\tilde{R}_{sin}(r)d^3r \underset{q\to\infty}{\approx} -\tilde{R}(0)\hat{D}\int e^{-i\mathbf{q}\cdot\mathbf{r}}U(r)d^3r \tag{4}$$

where the differential operator $\hat{D} = \varepsilon_{i\ldots n}\,(l, l_z)\,\partial/\partial q_i \ldots \partial/\partial q_n$, and μ is the reduced mass of the particles.

Eqs. (3) and (4) determine the asymptote of integral (2), and the asymptote of form-factor (1) for $q \to \infty$. In particular, for a transition between the states with the angular momenta $l_1 = 0$ and $l_2 = l$, we find:

$$eF_{0\to 1m} \approx -8(2i)^l \pi^{5/2}\frac{\mu}{\hbar^2}\tilde{R}_1(0)\tilde{R}_2(0)Y^*_{lm}\left(\frac{\mathbf{q}}{q}\right)\times$$
$$\times\left\{e_1\left[q_1^l\frac{\partial^l}{\partial\,(q_1^2)^l}\frac{\tilde{U}\,(q_1)}{q_1^2} + q_1^{l-2}\frac{\partial^l}{\partial\,(q_1^2)^l}\tilde{U}\,(q_1)\right] + (-1)^l e_2\,[q_1 \to q_2]\right\} \tag{5}$$

where the symbol $[q_1 \to q_2]$ means the expression written in the first square bracket, but with q_1 replaced by q_2, and

$$\tilde{U}(q) = \frac{1}{(2\pi)^3}\int U(r)e^{-i\mathbf{q}\cdot\mathbf{r}}d^3r$$

Note that the power-law decrease of the form-factors for $q \to \infty$ is similar to that mentioned in Problem 4.18 in connection with the asymptotes of the wavefunctions
in the momentum representation. In particular, for potentials such that $\tilde{U} \approx -\alpha/q^n$ with $n > 1$, the form-factor is

$$F_{1\to 2} \propto q^{-(2+n+l_1+l_2)} \text{ for } q \to \infty \tag{6}$$

To illustrate the result obtained, we consider the application of Eq. (5) to the hydrogen atom. In the approximation of an infinitely heavy nucleus, Eq. (5) must be slightly revised by simply putting $q_2 \equiv 0$. So, the term $e_2 e^{-i\mathbf{q}\cdot\mathbf{r}_2}$ in Eq. (1), which corresponds to the proton contribution, is now reduced to just its charge e, and inelastic transitions give no contribution to the form-factor due to the wavefunctions' orthogonality. Taking into account that for the Coulomb potential, $\tilde{U} = -e^2/2\pi^2 q^2$, and using the values of the radial functions at zero for this potential (given in Problem 13.79), we find for the transitions $1s \to ns$ and $1s \to np$ with $n \geq 2$:

$$F_{1s\to ns} \approx -\frac{16}{n^{3/2}\,(qa_B)^4}, \quad F_{1s\to npm} \approx \frac{16\sqrt{3}i\sqrt{n^2-1}\,(\varepsilon^*(m)\cdot\mathbf{q}/q)}{n^{5/2}\,(qa_B)^5}$$

These results, of course, coincide with the asymptotes of the exact expression for the form-factor, calculated in Problem 13.80.

GKKG.13.85

Find the differential and total cross-sections of Coulomb excitation of an atomic nucleus (initially in a state with the angular momentum, $J = 0$) by a fast, light, charged particle by a) dipole ($E1-$) and b) monopole ($E0-$) nuclear transition.

Solution

Just as in the previous problems, the sought-after cross-sections could be related to nuclear electric form-factors $F_{i\to f}(\mathbf{q}) = \langle f|\sum_p e^{-i\mathbf{q}\cdot\mathbf{r}_p}|i\rangle$ for the corresponding transitions. Summation is performed over all nuclear protons; $\mathbf{r}_p$ are their radius-vectors with respect to the nucleus' center of mass.

For non-relativistic collisions between the light particle and the nucleus, there holds the inequality $qr_p \leq pR/\hbar \ll 1$ (where R is the nucleus radius, and $p = mV$ is the incident particle momentum), so that in the expression for the form-factor, we can expand the exponent and keep only the first non-zero term. The differential cross-sections of the processes considered are $d\sigma_{E1}/dq^2 \propto q^{-2}$ and $d\sigma_{E0}/dq^2 = \text{const}$, while the total cross-sections are

$$\sigma_{E1} = \frac{8\pi e^2}{\hbar^2 V^2}\left|\langle J = 1, J_z = 0|\,d_z\,|0\right\rangle\right|^2 \ln\frac{p+p'}{p-p'} \tag{1}$$

(the cross-section is summed over projections of the angular momentum of the p-state; though the state has $J_z = 0$, we should take into account that the choice of the

[384] Assume that the (electron, muon) Compton wavelength $\hbar/mc$ is larger than the nuclear size, and the particle charge is $\pm e$.
quantization axis z along the vector $\mathbf{q}$ depends on the scattering angle; compare to Problem 13.80) and

$$\sigma_{E0} \approx \frac{4\pi}{9}\left(\frac{me^2}{\hbar^2}\right)^2 \frac{p'}{p}\,|Q_0|^2\,, \quad Q_0 = \langle f|\sum_p r_p^2|i\rangle \tag{2}$$

(parameter Q_0 also determines the probability of inner conversion for the corresponding nuclear transition; see Problems 11.68 and 11.69). In these relations, p' is the particle momentum after collision.

GKKG.13.86

Find a relation between the amplitudes and differential cross-sections for elastic scattering of a neutron on a proton and of a proton on a hydrogen atom (in the ground state). Neglect the interaction of the neutron magnetic moment with the electron.

Solution

Due to the smallness of the nuclear-force radius, the time of interaction between the proton and neutron is much smaller than the characteristic atomic time. So for the electron, the result of the interaction between the neutron and proton could be considered as a sudden change resulting in the velocity boost $\mathbf{V} = \hbar\mathbf{q}/m_p$ for the proton-nucleus. Therefore, the following relation between the amplitudes of the processes considered follows:

$$f_{nH}(E,q) \approx f_{np}(E,q)a(q) \tag{1}$$

where

$$a(q) = \int |\psi_0(r)|^2 \exp\left\{-\frac{i}{\hbar}m_e\mathbf{V}\cdot\mathbf{q}\right\} d^3r = \frac{1}{\left[1+(qm_e a_B/2m_p)^2\right]^2} \tag{2}$$

is the probability amplitude for the atom to remain in the ground state. (Compare to Problem 11.58; we note that $a(q)$ coincides with the atomic form-factor; see 13.80.)

Since $a(0) = 1$, then, using the optical theorem and relation (1), we conclude that the total cross-sections of the neutron scattering from a proton and from a hydrogen atom are the same. [385] As is seen from Eqs. (1) and (2), the differential cross-sections, $d\sigma/d\Omega = |f|^2$, start to differ only for $qa_B \gtrsim m_p/m_e$, which corresponds to neutron energies that are much larger than atomic (since $\hbar q \le 2p$).

GKKG.13.87

Find the scattering cross-section for heavy charged particles (for example, protons or ions) from neutral atoms with zero angular momentum. The velocities of the scattered particles are assumed to be much lower than the velocities of atomic electrons, but at the same time, $V \gg \hbar/Ma_B$, where M is the particle mass. Use the quasi-classical expression for the scattering cross-section (see Problem 13.51).

Solution

The energy of the interaction between the charged particle and the atom at large distances, $r \gg a_B$, has the form (polarization potential, see Problem 11.49)

$$U(r) = \frac{Ze(\mathbf{d}\cdot\mathbf{r})}{2r^3} = -\frac{1}{2}\beta\frac{(Ze)^2}{r^4} \tag{1}$$

where Ze is the particle charge, and β is the atomic polarizability. The calculation of the scattering cross-section by quasi-classical equation (see Problem 13.51)

$$\sigma = 4\pi\int_0^\infty \left\{1-\cos\left[\frac{1}{\hbar v}\int_{-\infty}^{\infty} U\left(\sqrt{\rho^2+z^2}\right)dz\right]\right\}\rho d\rho \tag{2}$$

for a power-law potential was performed in Problem 13.52. For polarization potential (1), it gives

[0][385] It is important that $m_H \approx m_p$. A completely different situation arises for neutron scattering from a proton bound in a molecule. In the case of a heavy molecule, $M \gg m_p$, the scattering cross-section for small energies from the bound proton is four times larger than the scattering cross-section from a free nucleon.

$$\sigma = \pi\Gamma\left(\frac{1}{3}\right)\left(\frac{\pi\beta Z^2 e^2}{4\hbar v}\right)^{2/3} \tag{3}$$

Let us make several comments about this result. As it follows from (3), distances essential in the scattering process are of the order $\rho_0 \sim \sqrt{\sigma} \sim v^{-1/3}$ (in atomic units), and we put $Z \sim 1$ and $\beta \sim a_B^3$ (such estimation follows from the condition that for $\rho \sim \rho_0$, the argument of the cosine, i.e., the quasi-classical phase, is of order 1 ; let us note that for $r \leq a_B$, Eq. (1) is not applicable, but in the problem conditions such distances do not play an essential role). To be able to use Eq. (1), these distances must be large, $\rho_0 \gg 1$, hence $v^{1/3} \ll 1$. (The condition, $\rho_0/v \gg \omega_{\text{at}}^{-1}$, that ensures the adiabaticity of the atomic electrons, is also fulfilled; when it is broken, dynamic excitation processes become essential for the atom, and the notion of an interaction potential loses its strict meaning.) On the other hand, the quasi-classical condition must also be fulfilled: $l \sim N\rho_0 v \gg 1$, so $v^{2/3} \gg 1/M$(M is the mass of the particle considered). So, Eq.(3) is valid if the conditions

$$\left(\frac{m_e}{M}\right)^{3/2} v_{at} \ll v \ll v_{at} \tag{4}$$

are fulfilled. Hence, the particle must be heavy, $M \gg m_e$ (for electrons, Eq. (3) is not applicable).

GKKG.13.88

Find the charge-exchange cross-section [386] for the collision of a slow, $v \ll v_{at}$, negative ion, A^-, with its atom, A. Consider the atom and ion to be in their S-states, and the ion's valence electron to be weakly bound (see Problem 11.28). The relative motion of atom and ion should be treated quasi-classically.

Solution

The specifics of the situation involving a resonant charge-exchange process, for the relative velocity of colliding particles $1/\sqrt{M} \ll v \ll 1$ (in atomic units, M is mass of atom or ion), is determined by following facts. 1) The charge-exchange cross-section is large, $\sigma_{\text{non-rez}} \gg \pi a_B^2$, i.e., large impact parameters are essential. 2) The atom's and ion's relative motion is quasi-classical, and we can only straight ballistic trajectories, since $Mv^2 \gg 1$.3) States of the "inner" electrons of the atom and ion do not change in the collision process, while the outer-shell electron can be viewed as being in the field of two zero-range potentials. 4) Due to the adiabaticity of the collision process (for the electron subsystem), only transitions between levels that are close in energy matter, that represent, the even (g) and odd (u) states of the quasi-molecular ion. Recall that for $R \to \infty$, these states are degenerate in energy. With decrease of distance, to $R_c = 1/\alpha$, the odd term goes to the continuous spectrum, and ionization becomes possible (see Problem 11.28). But during the process of charge-exchange, distances which are much larger than R_c are essential.

In the conditions mentioned, the wavefunction of the outer-shell electron for large distances $\mathbf{R}(t) = \boldsymbol{\rho} + \mathbf{v}t$ between atoms has the form:

$$\psi(r, \mathbf{R}, t) \approx \frac{1}{\sqrt{2}}\left\{\exp\left\{-i\int\limits_{-\infty}^{t} E_g dt\right\}\psi_g + \exp\left\{-i\int\limits_{-\infty}^{t} E_u dt\right\}\psi_u\right\} \tag{1}$$

where $E_{g,u}(R)$ and

$$\psi_{g,u} \approx \frac{1}{\sqrt{2}}\left\{\psi_0\left(\mathbf{r} - \frac{\mathbf{R}}{2}\right) \pm \psi_0\left(\mathbf{r} + \frac{\mathbf{R}}{2}\right)\right\}$$

are the energy and wavefunction of the even (odd) molecular terms on such distances, while $\psi_0(r)$ is the wavefunction of a bound state in an isolated zero-range potential (see Problem 4.10). Coefficients in the superposition, (1), were chosen so that for $t \to -\infty$, the wavefunction has the form $\psi \approx C(t)\psi_0(\mathbf{r} - \mathbf{R}/2)$, i.e., describes an electron, localized in the vicinity of one atom, which corresponds to the ion before collision. So for $t \to +\infty$, the coefficient in front of the wavefunction $\psi_0(\mathbf{r} + \mathbf{R}/2)$ determines the probability of charge-exchange:

[386] Compare to the charge-exchange cross-section in the collision between a slow proton and a hydrogen atom.

$$W_{ch-ex}(\rho) = \sin^2\left[\int\limits_{-\infty}^{\infty}\left(E_u(R) - E_g(R)\right)\frac{dz}{2v}\right] \tag{2}$$

$\left(R^2 = \rho^2 + z^2, z = vt\right)$; here the charge-exchange cross-section is

$$\sigma_{ch-ex}(v) = \int_0^\infty 2\pi\rho W_{ch-ex}(\rho)d\rho \tag{3}$$

Compare Eqs. (2) and (3) to the expression for the elastic scattering cross-section from a potential, $U(r)$, in the quasi-classical approximation, as considered in Problem 13.51.

According to Problem 11.28, at large distances, $E_u - E_g \approx 2\alpha e^{-\alpha R}/R$, where $\varepsilon_{\text{bind}} = \alpha^2/2$ is the binding energy of an electron in the ion. Writing

$$e^{-\alpha R} \approx \exp\left\{-\alpha\rho\left(1+\frac{z^2}{2\rho^2}\right)\right\}$$

we find that the integral in Eq. (2) in the case $\alpha\rho \gg 1$ is equal to

$$I(\rho) \approx \sqrt{\frac{2\pi\alpha}{\rho}}\frac{1}{v}e^{-\alpha\rho}$$

Due to its pronounced dependence on ρ, the argument of the sine in Eq. (2) decreases rapidly with an increase in ρ. Thus, the dominant contribution to integral (3) is in the region of impact parameter $\rho \leq \rho_0$ (where $I(\rho_0) = 1$), where the rapidly oscillating factor $\sin^2 I(\rho)$ could be replaced by its mean value, equal to 1/2. This gives

$$\sigma_{ch-ex}(v) \approx \frac{1}{2}\pi\rho_0^2 \approx \frac{\pi}{2\alpha^2}\ln^2\left[\frac{\alpha}{v}\sqrt{\frac{2\pi}{\ln\sqrt{2\pi\alpha^2/v^2}}}\right] \tag{4}$$

Note that the value ρ_0 satisfying equation $I(\rho_0) = 1$, which is convenient to write in the form $\ln I(\rho_0) = 0$, can be obtained by successive iterations. The first iteration gives $\alpha\rho_0 = \ln(\sqrt{2\pi}\alpha/v)$

Finally, we emphasize that the large value of the charge-exchange cross-section in Eq. (4) is due to the fact that for a weakly-bound electron, $\alpha \ll 1$.

GKKG.13.89

For the collision of identical atoms, one of which is in the ground state while the other is in an excited state (these states are connected by a dipole transition), estimate the interaction cross-section and, in particular, the excitation transfer cross-section. Consider the atoms' angular momenta to be equal to 0 and 1. The velocity of the atoms' relative motion is assumed to be small in comparison to the characteristic
atomic velocity, while the energy, on the other hand, is assumed to be much larger than atomic. Compare to the previous problem.

Solution

An important property of the process considered, that leads to a large excitation transfer cross-section (as well as to a large elastic scattering cross-section) is the neardegeneracy of the states corresponding to an excitation of one of the identical atoms if the distance between them is large. Therefore, for slow collisions, transitions between the close-in-energy states appear if the impact parameter is large enough. Interaction between the atoms, which has a dipole-dipole nature, was discussed in Problem 11.55. In comparison to the previous problem, here the difficulty arises due to an increase in the number of states: there are three g-terms and three u-terms. These are independent states corresponding to different polarizations of the excited atom (with the angular momentum $l = 1$).

One such state, which corresponds to the projection of the angular momentum $l_z = 0$ of the excited atom with the angular momentum $l = 1$, evolves independently of the other two. Here, as well as in the previous problem, the translational motion of atoms is considered quasi-classically in the approximation of a straight-line trajectory, and axis z is chosen perpendicular to the plane of motion. For this state, $U_{g,u} = \pm d^2/\left(3R^3\right)$ (see Problem 11.55), and calculation of the excitation transfer cross-section could be performed by Eqs. (2) and (3) from Problem 13.88. Calculating the integral

$$\int_{-\infty}^{\infty}\left[U_g(R) - U_u(R)\right]\frac{dz}{2v} = \frac{d^2}{3v}\int_{-\infty}^{\infty}\frac{dz}{\left(\rho^2+z^2\right)^{3/2}} = \frac{2d^2}{3\rho^2 v}$$

just as in the previous problem, we find the excitation transfer cross-section with $l_z = 0$:

$$\sigma_0 = \int_0^\infty 2\pi\rho\sin^2\left(\frac{2d^2}{3\rho^2 v}\right)d\rho = \frac{2\pi d^2}{3v}\int_0^\infty \sin^2 x\frac{dx}{x^2} = \frac{\pi^2 d^2}{3v} \tag{1}$$

As stated in the problem condition, it much exceeds the atomic length-scales (remember that $v \ll 1$).

For the two other polarized states of the excited atom (with $l_z = \pm 1$, or with $l_{x,y} = 0$; see Problem 3.21 and also Problem 3.41), calculation of the excitation transfer cross-section needs to rely on numerical methods. Note that in this case, transitions appear between such states, i.e., in the process of excitation transfer, the atom polarization may change. Diagonalization of the "instantaneous" Hamiltonian (performed in Problem 11.55) is based on the choice of a quantization axis along the direction, which passes through the atoms' centers. But due to their motion, the corresponding "rotating" system is non-inertial. Going to this rotating system gives rise to the following additional term in the Hamiltonian:

$$\hat{V}_{\text{cor}} = -\hat{\mathbf{\Omega}} \cdot \hat{\mathrm{l}} = -\frac{1}{I}\hat{L}_z\hat{l}_z = -\frac{v\rho}{R^2}\hat{l}_z$$

This is the Coriolis interaction, [387] (compare to Problem 6.29). The Coriolis operator does not commute with the operators of the "instantaneous" Hamiltonian, and this leads to transitions between the eigenstates, except for the case of $l_z = 0$ mentioned above. As for the estimation of the excitation transfer cross-section, it is evident that, as in Eq. (1), it is of order $\sigma \sim \pi d^2/v$.

GKKG.13.90 Elastic and inelastic scattering on black sphere

Find the total cross-section σ_{tot}, elastic cross-section σ_{el}, and inelastic cross-section σ_{in}, for the scattering of fast particles, $kR \gg 1$, from an absorbing ("black") sphere of radius R. Find also the differential cross-section of elastic scattering. Compare to Problems 13.57 and 13.58.

Hint: Use quasi-classical ideas to describe particle motion. Assume that all particles that reach the surface of the sphere are absorbed by it.

Solution by Kiselev

(У него это смотрел, возникнет вопрос - в первую очередь его и буду изучать)

Solution

Since we are dealing with a fully-absorbing "black" sphere, all scattering phases in Eq. $f(k,\theta) = \sum_{l=0}^{\infty}(2l+1)\varphi_l(E)P_l(\cos\theta)$; $\varphi_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{1}{k(\cot\delta_l - i)}$ for the amplitude of elastic scattering are the same: $\delta_l = i\infty\left(e^{2i\delta_l} = 0\right)$ for $l < l_0 = kR$ and $\delta_l = 0$ for $l > l_0$. Such values of δ_l correspond to the following physical picture (particle motion is quasi-classic, since $kR \gg 1$): particles with impact parameter $\rho = l/k < R$ are "absorbed" by the sphere, while those with $\rho > R$ move freely. Elastic scattering by its physical nature is analogous to Fraunhofer diffraction on an opaque screen (in this case, a fully absorbing screen). It is described by the scattering amplitude (compare to Problem 13.57)

$$f_{difr} = \frac{i}{2k}\sum_{l=0}^{l_0}(2l+1)P_l(\cos\theta) \approx \frac{iR}{\theta}J_1(kR\theta), \quad \theta \ll 1 \tag{1}$$

Using the optical theorem, we find total collision cross-section

$$\sigma_{tot} = \frac{4\pi}{k}\,\mathrm{Im}\, f_{difr}(\theta = 0) = 2\pi R^2 \tag{2}$$

The inelastic scattering cross-section (the absorption cross-section) is equal to

$$\sigma_{\text{inel}} = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\left(1 - |S_l|^2\right) = \frac{\pi}{k^2}\sum_{l=0}^{l_0}(2l+1) \approx \pi R^2 \tag{3}$$

while the elastic scattering cross-section is

$$\sigma_{el} = \sigma_{tot} - \sigma_{inel} \approx \pi R^2 \tag{4}$$

of inertia with respect to the center of mass. In the quasi-classical approximation, the operator $\hat{\mathbf{L}}$ could be replaced by the only non-zero component $L_z = \mu\rho v$.

This result is obtained by direct calculation of

$$\sigma_{el} = \int |f_{difr}|^2\, d\Omega = \pi R^2$$

just as in Problem 13.57.

GKKG.13.91

Interaction between an electron and a positron may result in their mutual annihilation, i.e., their conversion into a pair into photons. Because of this, positronium levels have a width, connected to the finite lifetime of the states (see Problem 11.61).

Find a relation between the level width, Γ_{ns}, for the s-states of positronium and the annihilation cross-section of a pair, $\sigma_{an}(v)$.

Hint: Taking into account the fact that the annihilation interaction radius is small, $R_{an} \sim \hbar/m_e c \ll a_B$, use perturbation theory in terms of the scattering length for the level shift and for the phase shift. See Problems 13.36 and 13.37.

Solution

Note that in the non-relativistic case, $kR_{an} \ll 1$. Thus annihilation processes are most important for the s-states. The effect of short-range interaction on an s-state is described by only one parameter: $a_0^{(S)}$, the scattering length (for the angular momentum, $l = 0$) of an isolated center (see Problems 13.36 and 13.37). For inelastic processes, the (annihilation) scattering length has a non-zero imaginary part. So, the level shift (see Problem 13.36) has an imaginary part, which determines the level width:

$$\Gamma_{ns} = -2\,\mathrm{Im}\,\Delta E_{ns} = -\frac{8\pi\hbar^2}{m_e}\left|\psi_{ns}^{(0)}(0)\right|^2 \mathrm{Im}\,a_0^{(S)} \tag{1}$$

Here, we have taken into account that for positronium, the reduced mass is $m = m_e/2$, and $\psi_{ns}^{(0)}(0)$ is the wavefunction at zero for the unperturbed state.

On the other hand, the change of the s-wave phase shift for the Coulomb potential, $U = -e^2/r$, under the influence of a short-range interaction, according to Problem 13.37 is equal to

$$\Delta\delta_0^{(S)}(k) = -\tilde{Q}_{k0}^2 k a_0^{(S)} \tag{2}$$

where

$$\tilde{Q}_{k0}^2 = \frac{\pi}{ka_B\left(1 - \exp\{-\pi/ka_B\}\right)}, \quad \left|\psi_{ns}^{(0)}(0)\right|^2 = \frac{1}{8\pi a_B^3 n^3} \tag{3}$$

and $a_B = \hbar^2/m_e e^2$. (In (3), the fact that the Bohr radius for positronium is twice as large as the atomic Bohr radius has been used.) From the phase shift of the elastic
scattering amplitude (its imaginary part), we find the annihilation cross-section:

$$\sigma_{an} = \frac{\pi}{k^2}\left(1 - |S_0|^2\right) = \frac{\pi}{k^2}\left(1 - \exp\left\{-4\,\mathrm{Im}\,\Delta\delta_0^{(S)}\right\}\right) \approx \frac{4\pi}{k^2}\,\mathrm{Im}\,\Delta\delta_0^{(S)} = \\ = -\frac{4\pi}{k^2}\tilde{Q}_{k0}^2\,\mathrm{Im}\,a_0^{(S)} \tag{4}$$

According to Eqs. (1) and (4), we obtain:

$$\Gamma_{ns} = \hbar\left|\psi_{ns}^{(0)}(0)\right|^2 \frac{1}{\tilde{Q}_{k0}^2}\left(v\sigma_{an}(v)\right) \tag{5}$$

where $v = \hbar k/m = 2\hbar k/m_e$ is the relative velocity of the electron-positron pair. In the case $\hbar v/e^2 \gg 1$, when the Coulomb potential could be considered as a perturbation, relation (5) becomes simpler, since here $\tilde{Q}_{k0}^2 \approx 1$.

In conclusion, we emphasize that both the annihilation cross-section and positronium level widths (and hence their lifetime $\tau = \hbar/\Gamma$) depend strongly on the value of the total electron-positron pair spin (see Problem 11.61), so that the ortho- and para-states of the positronium should be considered separately. Let us also mention that these results could be extended to describe hadron atoms. However, the condition of their applicability assumes that there is no s-level with small binding energy in the strong short-range potential. See Problem 11.4, and also Problem 11.74.

GKKG.13.92

Using the principle of detailed balance, relate the cross-section of neutron radiation capture by a proton, $n + p \to d + \gamma$, and the cross-section of photodisintegration of a deuteron, $d + \gamma \to n + p$

Hint: The relation between cross-sections of mutually inverse two-particle processes, which appear in the principle of detailed balance, is valid in the relativistic region as well. Keep in mind that although the photon spin is equal to 1, it has only two independent polarizations.

Solution

According to the principle of detailed balance for inverse reactions $A \to B$ and $B \to A$, the relation

$$\frac{\bar{\sigma}_{A\to B}}{\bar{\sigma}_{B\to A}} = \frac{g_B p_B^2}{g_A p_A^2} \tag{1}$$

must be satisfied. Here $\bar{\sigma}$ are total cross-sections of the corresponding reactions $A \to B$ and $B \to A$, averaged over the particle spins in the initial state, and summed over the particle spins in the final state; $g_{A,B}$ are the spin statistical weights, and $p_{A,B}$ are the momenta of relative motion in two-particle systems A and B, taken at the same
energy in the center-of-mass system (analogous relations hold not only for the total but also for the differential reaction cross-sections).

In the case of the reactions, $n + p \rightleftharpoons d + \gamma$ we have $\sigma_{A\to B} \equiv \sigma_{\text{cap}}$ (neutron radiation capture cross-section) and $\sigma_{B\to A} \equiv \sigma_{ph}$ (deuteron photodisintegration cross-section). Since the spin (polarization) statistical weight for a particle with spin s is equal to $g_s = (2s+1)$ (except for the photon, for which $g_\gamma = 2$ due to its transverse polarization), then

$$g_A = (2s_p + 1)(2s_n + 1) = 4, \quad g_B = g_\gamma (2s_d + 1) = 6 \tag{2}$$

Momenta $p_{A,B}$ in Eq. (1) are equal to the momenta of the particles in the rest frames of systems A, B. For the reactions considered, $p_A \equiv p_p = p_n$ and $p_0 \equiv p_\gamma = p_d$. Considering all particles to be non-relativistic (except for the photon; for it we have $E_\gamma \ll Mc^2$, where M is the mass of a nucleon), then according to the energy conservation law we obtain

$$E_A = \frac{1}{M} p_A^2 = E_B = E_\gamma + E_d - \varepsilon_0 \approx \hbar\omega - \varepsilon_0$$

We have defined by ε_0 the deuteron binding energy and by ω the photon frequency. We have neglected the value E_d in comparison to E_γ (for a non-relativistic deuteron, $E_d \ll E_\gamma$ for $p_d = p_\gamma$).

Taking into account the fact that $p_\gamma = \hbar\omega/c$, according to Eqs. (1)-(3) we find:

$$\frac{\sigma_{cap}}{\sigma_{ph}} = \frac{3}{2} \frac{\hbar\omega}{Mc^2} \frac{\hbar\omega}{\hbar\omega - \varepsilon_0} \tag{4}$$

Thus, it follows that in the non-relativistic case, $\hbar\omega \ll Mc^2$, we have $\sigma_{ph} \gg \sigma_{\text{cap}}$. The only exception is a narrow region of values $\hbar\omega$ in the vicinity of the reaction $d + \gamma \to n + p$ threshold (here $\hbar\omega \approx \varepsilon_0$), where, conversely, $\sigma_{ph} \ll \sigma_{cap}$.

In conclusion, we emphasize that Eq. (4), as well as Eq. (1), does not rely on any information or assumptions about the mechanism(s) driving the reaction, but is based solely on the symmetry of quantum mechanical equations with respect to time-reversal.

GKKG.13.93

Find the relation between the cross-section of photoelectric effect (a.k.a. "photoeffect") from the ground state of a hydrogen atom and the radiation recombination cross-section of an electron with a proton (the process inverse to photoeffect) into the ground state of a hydrogen atom.

Solution

This problem is solved similarly to the previous one (moreover, the processes considered in these two problems are physically related; see also Problems 14.38 and 14.19). Averaged over the spins, the cross-sections of the photoeffect reaction, $\gamma + H \to e + p$, and the radiation recombination reaction, $e + p \to H + \gamma$, are connected by the relation:

$$\frac{\sigma_{ph}(\omega)}{\sigma_{rec}(\varepsilon_e)} = \frac{p_e^2}{2p_\gamma^2} = \frac{\hbar\omega - |E_0|}{\hbar\omega} \frac{m_e c^2}{\hbar\omega} \tag{1}$$

To prove Eq. (1), we should take into account that first, the center-of-mass frames for these reactions are the rest frames of the hydrogen atom in the ground state [388] or the proton; second, the statistical spin weight is equal to 4 for both the hydrogen atom and the electron-proton system. Finally, the electron and photon energies are connected by the energy conservation law as follows:

$$\hbar\omega + E_0 = \varepsilon_e = \frac{1}{2m_e} p_e^2$$

where E_0 is the energy of the hydrogen atom in the ground state.

[388] Here we neglect the hyperfine structure of the hydrogen atom (see Problem 11.2). Let us also note that for processes involving the hydrogen atom in a state with the angular momentum, l, the "spin" statistical weight is equal to $4(2l + 1)$.

17.5 Checking Basic Understanding

17.5.1 Questions on Understanding the Basics of Quantum Mechanics

Вопросы на понимание излучения, лазеров, ЭПР и ЯМР

- Какова пространственная четность электрических и магнитных фотонов? Как отличаются вероятности их испускания?
- Какие ещё четности Вам встречались в 5 семестре? Чем отличаются в этом контексте бозоны от ферминов?
- Чему пропорционален сигнал при магнитном резонансе?
- Почему ЯМР более распространён в практических приложениях, чем ЭПР?
- Почему трёхуровневая схема лазера работает плохо, а двухуровневая - совсем не работает?
- В чём отличие мазеров от лазеров?
- Какие мощности и энергии лазерного излучения достижимы на современном этапе?

17.5.2 Questions on Understanding Typical Sections of Quantum Mechanics

Вопросы на понимание основ ядерной физики

- Какие частицы считаются ядерноактивными, а какие - нет?
- Что такое сечение и выход ядерной реакции?
- Нарисовать качественно зависимость сечения радиационного захвата от энергии нейтрона для тяжёлого и лёгкого ядра
- По сравнению с чем сечение в один барн - это много или мало (указать примеры реакций)?
- В каком диапазоне энергий работает модель составного ядра?
- Почему энергетические ширины каналов реакции можно складывать?
- Чем удобна «перечёркнутая» дебройлевская длина?
- Как объясняет закон Бэте классическая и квантовая физика?
- Какими способами эволюционируют нестабильные ядра (лёгкие и тяжёлые) внутри долины стабильности?
- Для каких ядер (четно-четных, нечетно-четных, нечетнонечетных) закон Гейгера-Неттола выполняется лучше и почему?
- Почему спектры частиц при альфа-распаде дискретные, а при бета-распаде - непрерывные?
- Что является объектом бета-распада: ядро, нуклон или кварк?
- С какой точностью и как осуществляется радиоизотопная датировка?
- Что такое «вековое равновесие» изотопов?

17.5.3 Questions on Understanding Typical Details

Van-Riet. Commutator $[x, p]$ (????)

Let's consider $\langle p|[\hat{p}, \hat{x}]|p\rangle$. If we write

$$\langle p|[\hat{p}, \hat{x}]|p\rangle = \langle p|(\hat{p}\hat{x} - \hat{x}\hat{p})|p\rangle = (\langle p|\hat{p})\hat{x} - \hat{x}(\hat{p}|p\rangle) = p\hat{x} - p\hat{x} = 0$$

But also

$$\langle p|[\hat{p}, \hat{x}]|p\rangle = \langle p|(-i\hbar)|p\rangle = -i\hbar$$

Why?

Solution.

(напишу потом, важно понимать, что с.з. не эрмитовых матриц не переставляются, как в 1 случае. про это же строчка в 1й части.)

me. Bound and not Bound States

In 1D and in 2D, if there is an infinitesimal attraction, there ia a bound state. But in 3D, even though there is an equation for a radial motion, which has only one parameter, there is no bound state if the potential is not large enough. Why?

Solution.

One can say that there is an effective potential, thus for the radial equation there will be a different equation. But for the harmonic $l = 0$, there is no it, so the question remains.

(?? one can somehow use variational theorem, and see that there is not enough potential energy for a kinetic energy. (??? I'll try later. Don't know at the moment, how))

Answer is that the radial 3D Schrodinger equation is written for function $u(x)$, which is a part of the whole wavefunction $\psi(r) = u(r) \cdot r$ (?? check!!). Thus, the wavefunction will have a node in the center and it first grows fast (????), thus, there should ba a strong potential, to make it decreasing.

(point out that it will play an important role in discussing superconductivity)

ПТФ-3.y1 Вероятности по волновой функции (??)

Состояние трёхмерной частицы описывается нормированной волновой функцией $\psi(x, y, z)$. Какова вероятность того, что частица находится в интервале $z_1 < z < z_2$, а её импульс при этом - в интервале $p_1 < p_y < p_2$?

Solution.

$$\Psi(x, p_y, z) = \int\limits_{-\infty}^{\infty} dy e^{-\frac{ip_y y}{\hbar}} \psi(x, y, z)$$

$$\rho = |\Psi(x, p_y, z)|^2 = \left| \int\limits_{-\infty}^{\infty} dy e^{-\frac{ip_y y}{\hbar}} \psi(x, y, z) \right|^2$$

$$P = \int\limits_{-\infty}^{\infty} \int\limits_{p_1}^{p_2} \int\limits_{z_1}^{z_2} dx \frac{dp_y}{2\pi\hbar} dz \rho = \int\limits_{-\infty}^{\infty} \int\limits_{p_1}^{p_2} \int\limits_{z_1}^{z_2} dx \frac{dp_y}{2\pi\hbar} dz \left| \int\limits_{-\infty}^{\infty} dy e^{-\frac{ip_y y}{\hbar}} \psi(x, y, z) \right|^2$$

(?? как это связано с соотношением неопредленности? если так думать про в.ф., то будет ли оно выполняться?)

17.5.4 Typical Problems on Testing Knowledge of Quantum Models

17.5.5 Problems about Understanding States, Entanglement Measurements (???)

(это же в кв теор инфо. тут много всего будет потом)

ПТФ-2.з.? Отличие классической запутанности от квантовой

Есть две системы: $\hat{\rho}_{AB} = |\psi_{AB}\rangle\langle\psi_{AB}| = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$ и $\hat{\rho}_{AB} = \frac{1}{2}\left(\hat{\mathbb{P}}_{\uparrow\downarrow} + \hat{\mathbb{P}}_{\downarrow\uparrow}\right) = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$. Придумайте эксперимент, который мог бы их различить, если мы можем наблюдать только A ее часть.

Solution..

(нужно переучивать измерения, пока я не знаю это)
Экспериментатор C должен смотреть на результаты от первой и второй системы, далее посчитать среднее какого-то оператора в случае первой и второй системы.
так как в общем виде оно имеет вид

$$\langle O\rangle = \mathrm{Tr}(\hat{\rho}\hat{O}) = \underbrace{\sum_n \rho_{nn}\langle O\rangle_n}_{\text{classical statistics}} + \underbrace{\sum_{m\neq n} \rho_{nm}\langle m|\hat{O}|n\rangle}_{\text{quantum interference terms}} ,$$

то одина система даст только первое слагаемое, а вторая - что-то большее.
таким образом, система, у которой среднее значение оператора больше - квантовая.

ПТФ-2.у2. (10 б). Отличие запутанности от распутанности

Предположим, наблюдатель C хочет придумать эксперимент, который сможет отличить состояние «ЭПР» от классически запутанного («Носки») (из семинара). Какую наблюдаемую ему нужно придумать? Выразите её через матрицы Паули (и их тензорные произведения)?

Solution.

Наблюдаемая – гамильтониан из задачи 2 семинара 1:

$$\hat{H} = -J(\hat{\sigma}_1^x \otimes \hat{\sigma}_2^x + \hat{\sigma}_1^y \otimes \hat{\sigma}_2^y + \hat{\sigma}_1^z \otimes \hat{\sigma}_2^z)$$

Для “ЭПР”:

$$\mathrm{tr}(\hat{\rho}_{AB}\hat{H}) = \mathrm{tr}\left(\frac{J}{2}\begin{pmatrix}0&0&0&0\\0&1&1&0\\0&1&1&0\\0&0&0&0\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix}\right) = \mathrm{tr}\left(\frac{1}{2}\begin{pmatrix}0&0&0&0\\0&1&1&0\\0&1&1&0\\0&0&0&0\end{pmatrix}\right) = J$$

Для “Носок”:

$$\mathrm{tr}(\hat{\rho}_{AB}\hat{H}) = \mathrm{tr}\left(\frac{J}{2}\begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&0\end{pmatrix}\begin{pmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{pmatrix}\right) = \mathrm{tr}\left(\frac{J}{2}\begin{pmatrix}0&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&0\end{pmatrix}\right) = -J$$

Как видно, следы не совпадают. Искомая наблюдаемая:

$$\hat{H} = -J(\hat{\sigma}_1^x \otimes \hat{\sigma}_2^x + \hat{\sigma}_1^y \otimes \hat{\sigma}_2^y + \hat{\sigma}_1^z \otimes \hat{\sigma}_2^z)$$

17.5.6 Short Problems on Understanding Atoms

МФТИ.КР.2023.общеф-1/3. Прямое рассеяние

Фотон рассеивается на электроне, летящим перпендикулярно направлению фотона. Найти энергию электрона после столкновения если длина волна λ при рассеянии фотона назад не изменилась. m - масса электрона.

Solution..

(я хз, для начала обычные задачи дорешать нужно, потом мб дойду до такого)

МФТИ.КР.2023.общеф-2/3. Шаблон волновой функции

Волновая функция одного из состояний атома водорода имеет вид $\psi = A(1+\alpha r)e^{-\beta r}$, где A, α, β - некоторые константы. Определите величину констант, энергию основного состояния и квантовые числа.

Solution..

(хорошая задача, нужно сперва потренироваться еще)

МФТИ.КР.2023.общеф-3/3. Максимальное ядро

Оценить заряд ядра Z водородоподобного иона, начиная с которого невозможны стационарные электронные орбиты. Учесть, что для больших Z существенна релятивистская зависимость энергии от импульса.

Solution..

(хорошая задача, нужно сперва потренироваться еще)

17.5.7 Typical Problems on Testing Mastery of Methods

Feigelman.EntrExam.th-1/8

Weak electric field $\mathcal{E}$ is suddenly applied to a hydrogen atom. Find probability of transition into the nearest excited level.

Solution.

(???)

Feigelman.EntrExam.th-3/8

Particle with mass m is moving in 2D space in the field of repulsive potential $U(r) = W/r^2$. Assuming $\epsilon = 2mW/\hbar^2$ to be small, calculate full scattering " crosssection" with an accuracy up to ϵ^2 inclusive.

Solution.

(???)

Feigelman.EntrExam.th-4/8

Particle with strongly anisotropic spectrum $E = \frac{p_x^2}{2m_1} + \frac{p_x^2+p_y^2}{m_2}$, $m_1 \gg m_2$, is moving in the attractive potential $U(r) = -\alpha/r$. Find few low-lying energy levels.

Solution by Oleg Baburin.

(???)

Feigelman.EntrExam.th-5/8

Single quantum particle with a mass m is bound between walls with a distance L between them. Temperature T is high in the sense that $T \gg \hbar^2/mL^2$. Find quantum corrections to the "equation of state" which determine dependence of pressure on temperature $P(T)$.

Solution.

(???)

18 Other Problems about Basic Atomic Physics

18.1 Photons, Atoms, Molecules

(подробнее - в отдельных записях)

18.1.1 Problems about photons 1

(скорее всего выше это поставлю, типичные задачи)

О3.1-1.1(1 мин) Импульс фотона

Найти импульс фотона видимого света ($\lambda = 500$ нм). Сравнить его с импульсом молекулы водорода при комнатной температуре.

1.

1. Импульс фотона $p = \frac{\hbar\omega}{c} = \frac{2\pi\hbar}{\lambda} \approx 1,3 \cdot 10^{-22}\Gamma \cdot \text{с/с}$. Среднеквадратичный импульс молекулы водорода $p = \sqrt{3kTM} \approx 5,4 \cdot 10^{-19}\Gamma \cdot \text{ см/с}$.

О3.1-1.2(1 мин) импульс фотона

При какой длине волны импульс фотона равен импульсу молекулы водорода при комнатной температуре?

1.

2. $\lambda \approx 0,12\text{НМ}$.

О3.1-1.3(2 мин) поток фотонов (!???!?!??!?)

Излучение гелий-неонового лазера мощностью $W = 1$ мВт сосредоточено в пучке диаметром $d = 0,5\text{см}$. Длина волны $\lambda = 0,63$ мкм. Определить плотность потока j фотонов в пучке.

1.

3. $j = \frac{2W\lambda}{\hbar c\pi^2 d^2} \approx 1,7 \cdot 10^{16} \frac{\text{фотон}}{\text{с}^2 \cdot \text{с}}$.

О3.1-1.4 Проверяем ОТО (???)

Согласно общей теории относительности энергия любого объекта в статическом гравитационном поле $\mathscr{E} = \mathscr{E}_0 \left(1 + 2\varphi/c^2\right)^{-1/2}$, где $\mathscr{E}_0$-энергия объекта в «пустом» (т. е. свободном от гравитационных полей) пространстве, а φ - гравитационный потенциал в точке нахождения объекта. Показать на основе этого соотношения, что разница энергий $\Delta\mathscr{E} = \mathscr{E}_2 - \mathscr{E}_1$ между двумя состояниями объекта, расположенного на поверхности Земли и на высоте от нее, оказывается эквивалентной разнице «гравитационных энергий» излученного объектом γ-кванта с энергией $\mathscr{E}_\gamma = \mathscr{E}_2 - \mathscr{E}_1$ и массой $m_\gamma = \mathscr{E}_\gamma/c^2$, как это было показано в опытах Паунда и Ребки с помощью эффекта Мессбауэра.

1.

4*: Решение. Рассмотрим атом (ядро) в статическом гравитационном поле. Согласно условию задачи разность энергий $\Delta\mathscr{E}$ между основным и возбужденным состоянием зависит от положения атома (ядра) в гравитационном поле Земли

$$\Delta\mathscr{E} = \mathscr{E}_2 - \mathscr{E}_1 = \left(\mathscr{S}_2^0 - \mathscr{E}_1^0\right)\left[1 + \frac{\varphi(r)}{c^2}\right]^{-1/2} \tag{1}$$

где $\mathscr{E}_2^0$ и $\mathscr{E}_1^0$ - энергии уровней в «пустом» пространстве. Таким образом, наблюдатель на поверхности Земли обнаружит, что энергия излучения атома (ядра), находящегося на высоте H над поверхностью Земли (радиус R_3), не совпадает с таковой у поверхности, и наоборот. Именно это и было обнаружено в экспериментах Паунда и Ребки. При этом

$$\Delta\mathscr{E}\left(R_3+H\right)=\Delta\mathscr{E}\left(R_3\right)\sqrt{\frac{1+2\varphi\left(R_3\right)/c^2}{1+2\varphi\left(R_3+H\right)/c^2}}\approx$$

$$\approx\Delta\mathscr{F}(\mathscr{R})[+\frac{\varphi(\mathscr{R})-\varphi(\mathscr{R}+\mathscr{H})}{}] \tag{2}$$

Здесь мы учли, что гравитационный потенциал Земли слабый:

$$\frac{2\varphi\left(R_3\right)}{c^2}=\frac{2\gamma M_3}{R_3c^2}=2\cdot10^{-9}\ll1$$

Наивное (но неверное, хотя и часто используемое) объяснение наблюдае мого эффекта смещения уровней состоит в том, что γ-кванту с энергией $\mathscr{E}$ приписывается гравитационная масса $m_\gamma=\mathscr{E}/c^2$, после чего для фотона применяется нерелятивистская формула $\Delta\mathscr{E}=-m_\gamma\Delta\varphi$ (так же, как для какогонибудь камня). Фотон (как и камень) ускоряется; относительное изменение его энергии

$$\frac{\Delta\mathscr{E}}{\mathscr{E}}=-\frac{\Delta\varphi}{c^2} \tag{3}$$

Это полностью совпадает с результатом (2):

$$\frac{\Delta\mathscr{E}}{\mathscr{E}}\approx\frac{\Delta\varphi}{c^2}=\frac{\gamma M_3}{c^2R_3}H=\frac{gH}{c^2}.$$

Следует подчеркнуть, что согласно ОТО ход времени зависит от величи ны гравитационного потенциала. Иначе говоря, если ввести мировое время τ_0, измеряемое часами в отсутствии гравитационных полей, то в точке с по тенциалом $\varphi(r)$ ход часов меняется:

$$\boldsymbol{\tau}=\tau_0\left(1+\frac{2\varphi(r)}{c^2}\right)^{-1/2}$$

Это означает, что наблюдатель в точке с нулевым потенциалом видит, что частота света в любом месте одинакова, а скорость света меняется, и стати ческое гравитационное поле эквивалентно среде с показателем преломления n (см. задачу 1.5). Для наблюдателя, находящегося в ненулевом потенциале, частота (т.е. прошедшее мимо него за единицу времени число «горбов», явля ющееся инвариантом) изменилась. Однако скорость света в его системе равна c.

Отметим, что можно говорить о «красном смещении» фотона по отношению к наблюдателю в точке с нулевым гравитационным потенциалом, если относить это не к частоте, а к длине волны (импульсу) фотона.

О3.1-1.5 Гравитационное отклонение через аналогию с показателем преломления (??)

Как следует из общей теории относительности, статическое гравитационное поле по отношению к своему воздействию на электромагнитные волны эквивалентно неоднородной среде с показателем преломления $n=\left(1+2\varphi/c^2\right)^{-1}$, где φ - гравитационный потенциал. Используя эту аналогию, найти угол отклонения ∂ луча света при прохождении его вблизи края Солнца. Масса Солнца $M=1,99\cdot10^{33}$г, радиус его фотосферы $R=696000$ км.

1.

5. $\delta=\frac{4\gamma M}{Rc^2}\approx0,84\cdot10^{-5}$ рад $=1,75''$.

Гравитационный потенциал Солнца на расстоянии r от него $\varphi(r)=-\gamma M/r$. Если обозначить через α угол падения луча света, т. е. угол между лучом света, упавшим на слой «среды» толщиной dr, и радиальным направлением к центру Солнца, то согласно закону Снеллиуса

$$\frac{\sin(\alpha-d\alpha)}{\sin\alpha}=\frac{n(r-dr)}{n(r)}$$

где $\alpha-d\alpha$ - угол преломления луча света гравитиационным полем. Отсюда следует, что $\operatorname{ctg}\alpha d\alpha=\frac{d}{dr}\ln n(r)$. В силу того, что гравитационный потенциал Солнца мал, легко установить, что $\ln n(r)\approx\frac{2\gamma M}{c^2r}$ и $dr=-\frac{R\cos\alpha}{\sin^2\alpha}d\alpha$. Таким образом, искомый угол поворота луча света δ равен удвоенному углу отклонения на пути из бесконечности ($\alpha=\pi/2$) до $R(\alpha=0)$ (в силу обратимости световых лучей):

$$\delta = -\frac{4\gamma M}{c^2 R}\int_{\pi/2}^{0}\sin\alpha d\alpha$$

откуда и следует ответ.

(????? насколько полезен такой метод показателя преломления????)

О3.1-1.6 Преломление фотонов

Исходя из классического закона преломления света, показать, что при прохождении плоской границы двух прозрачных сред сохраняется тангенциальная компонента импульса фотонов.

О3.1-1.7 Выбивание фотонов

Электромагнитная волна с круговой частотой $\omega = 2\cdot 10^{16}\text{с}^{-1}$ промодулирована по амплитуде синусоидой с круговой частотой $\Omega = 2\cdot 10^{15}\text{с}^{-1}$. Найти энергию фотоэлектронов, выбиваемых этой волной из атомов водорода с энергией ионизации $_{\text{n}} = 13,5$ эВ.

Solution

(?? вспомнить разложение в спектр???)
1.7. $\mathscr{E} = \hbar(\omega+\Omega) - \mathscr{E}_{\text{и}} \approx 0,9$ эВ.

О3.1-1.8 Рентгеновская трубка (???)

Найти напряжение V на рентгеновской трубке, если известно, что в излучаемом ею сплошном спектре нет длин волн, меньших 0,0206 нм.

Solution

(?? вообще хз, что за трубка??? нужна строчка про нее в 1 части.)
1.8. $V = 60\text{кВ}$.

О3.1-1.9

Шарик электроскопа облучается монохроматическим рентгеновским излучением. Листочки электроскопа перестают расходиться, когда потенциал шарика равен 8 кВ. Определить длину волны λ падающего излучения.

1.

9. $\lambda = 0,154$ нм.

О3.1-1.10

В центре посеребренного изнутри вакуумного стеклянного баллона шаровой формы помещен маленький шарик, покрытый никелем. Шарик освещается светом от ртутной лампы с длиной волны $\lambda = 230,2$ нм. Между внутренней поверхностью сферы и шариком приложена задерживающая разность потенциалов. Оказалось, что при увеличении этой разности до $V = 0,75$ В ни один из фотоэлектронов не попадает на посеребренную поверхность сферы. Контактная разность потенциалов между никелем и серебром равна $V_{\mathbb{K}} = 1$ В. Вычислить максимальную скорость фотоэлектронов.

1.

10. $v_{\max} = \sqrt{2e\left(V+V_{\text{K}}\right)/m_{\text{e}}} = 784\text{к/с}$.

О3.1-1.11 Максимальная зарядка шара светом (!)

Уединенный цинковый шарик облучается ультрафиолетовым светом с длиной волны $\lambda = 250$ нм. До какого максимального потенциала зарядится шарик? Работа выхода электрона для цинка $A = 3,74$ эВ.

1.

11. $V = \frac{(hc/\lambda)-A}{e} = 1,23$ В.

Пишем формулу фотоэффекта (????)
(??? подумаю еще про это.)

О3.1-1.12

При каких длинах волн λ облучающего света шарик в условиях предыдущей задачи заряжаться не будет?

1.

12. $\lambda > 2\pi\hbar c/A \approx 331$ нм.

О3.1-1.13 Фотоэлемент с разностью потенциалов (!?!???)

Цинковый электрод вакуумного фотоэлемента освещается монохроматическим светом с длиной волны $\lambda = 250$ нм. При наложении задерживающей разности потенциалов фототок уменьшается и обращается в нуль, когда она достигает значения $V = 2$ В. Определить внешнюю контактную разность потенциалов $V_{\text{к}}$ между цинком и материалом, из которого изготовлен другой электрод фотоэлемента. Работа выхода электрона из цинка $A = 3,74$ эВ.

Solution

(???? думаю, хорошая задача на проверку. лучше по Корявову пока буду решать, я пока тупой, вряд ли правильно решу.)

О3.1-1.16 Электрон только рассеивает (!?!?!??!?!?!?)

Показать, что свободный электрон в вакууме не может ни поглощать, ни излучать фотоны, а лишь рассеивать их.
(!??!? что, почему??)

О3.1-1.17 Максимальный фототок

Какую минимальную длительность импульса фототока можно получить в вакуумном фотоэлементе, между анодом и фотокатодом приложено напряжение $E = 300$ В/см, при освещении фотокатода короткими ($< 10^{-11}$с) импульсами света с длиной волны $\lambda = 500$ нм. Красная граница материала фотокатода $\lambda_{\text{кр}} = 1000$ нм.

Solution

У нас просто по формуле Эйнштейна выбивается электрон, а дальше он ускоряется в постоянном поле. Длительность импульса - длительность во времени, привыкаем к общефизическим словам.
Максимальная скорость выбиваемых электронов

$$\frac{mV_{\max}^2}{2} = h(\omega - \omega_0) = hc\left(\frac{1}{\lambda} - \frac{1}{\lambda_0}\right)$$

$$V_{\max}^2 = \frac{2hc}{m}\left(\frac{1}{\lambda} - \frac{1}{\lambda_0}\right)$$

Кинематическая задачка о времени пролета электронов в трубке длиной I:

$$I = \frac{eEt_1^2}{2m} = V_{\max}t_2 + \frac{eEt_2^2}{2m}$$
$$t_1 = t_2\sqrt{1 + \frac{2mV_{\max}}{eEt_2}} \approx t_2 + \frac{mV_{\max}}{eE}$$

где мы разложили корень, потому что значение добавки мало. В итоге:

$$\Delta t = t_1 - t_2 = \frac{1}{eE}\sqrt{\frac{2hc}{m}\left(\frac{1}{\lambda} - \frac{1}{\lambda_0}\right)} = 1.2 \cdot 10^{-10}\text{с}.$$

(еще раз подумаю про это потом)

О3.1-1.18 Накопление энергии для фотоэффекта (???)

По классической электромагнитной теории света поток световой энергии от источника непрерывно распространяется во все стороны. Через какой промежуток времени, согласно этой теории, отдельный атом танталового катода может накопить столько энергии, чтобы стал возможен вылет фотоэлектрона, если катод находится на расстоянии $L = 10$ м от 25-ваттной лампочки? Работа выхода электрона для тантала составляет $A = 4$ эВ. Считать, что фотоэлектрону передается вся энергия, накапливающаяся в атоме тантала, диаметр которого можно считать равным $d = 0,3$ нм.

Solution

(??? это ведь неверно, так же не происходит??? накопление какое-то???)

О3.1-1.19

Исходя из представления о фотонах как о квантах света, вывести формулу для эффекта Доплера в предположении, что источник света движется с нерелятивистской скоростью.

О3.1-1.20

То же, но для источника, движущегося с релятивистской скоростью.

О3.1-1.22

На рис. 2 (!!?!??!!?!!) изображены результаты, полученные Комптоном при исследовании рассеяния рентгеновских лучей в графите. Наблюдения велись под углом $\theta = 135^\circ$ к направлению падающего пучка. Определить длину волны λ_0 падающего излучения.

О3.1-1.23

Фотон рентгеновского излучения с длиной волны λ в результате комптоновского рассеяния на неподвижном свободном электроне отклонился от первоначального направления на угол θ. Определить кинетическую энергию T_e и импульс p_e электрона отдачи. Дать численный ответ для $\lambda = 0,02$ нм и $\theta = 90^\circ$.

Solution

(?? следствие ур Комптона)

О3.1-1.24

В предыдущей задаче определить угол φ между направлением первичного фотона и направлением движения электрона отдачи.

О3.1-1.25

Определить изменение длины волны при эффекте Комптона, если наблюдение ведется перпендикулярно к направлению первичного пучка излучения.

О3.1-1.26 Возможный угол вылета (???!!!!?)

В результате комптоновского рассеяния фотона на покоящемся электроне последний получил импульс отдачи p. Определить, под какими углами по отношению к направлению падающего фотона мог вылететь электрон с таким импульсом.

Solution

Используя векторную диаграмму рис. 1.8 (вставлю потом) и теорему косинусов, получаем

$$(hv_1/c)^2 = (hv/c)^2 - 2(hv/c)p\cos\varphi + p^2.$$

Вводя кинетическую энергию электрона после соударения $T = E - mc^2$, где E - энергия электрона после соударения, а m - его масса покоя, из закона сохранения энергии имеем $hv_1 = hv - T$. Подставляя это в предыдущее уравнение (исключая hv_1), находим

$$hv = \frac{1}{2}\left(p^2c^2 - T^2\right)/(pc\cos\varphi - T)$$

Используя выражение для T и связь энергии с импульсом $E^2 = p^2c^2 + m^2c^4$, получаем, что числитель - положительная величина. Так как hv также положительная величина, то и знаменатель выражения для hv должен быть положительной величиной:

$$pc\cos\varphi - T > 0,$$

откуда

$$\cos\varphi > T/(pc) = \left[1 + (mc/p)^2\right]^{1/2} - mc/p.$$

Таким образом, диапазон углов, под которыми мог вылететь электрон с заданным импульсом, лежит в пределах

$$0 < \varphi < \arccos\left[\left(1 + m^2c^2/p^2\right)^{1/2} - mc/p\right]$$

О3.1-1.27

В результате комптоновского рассеяния фотона на покоящемся электроне последний вылетел под углом $\alpha = 60°$ к направлению падающего фотона. Какую максимальную кинетическую энергию T может приобрести электрон отдачи в этом случае?

О3.1-1.28

В результате комптоновского рассеяния фотона на покоящемся электроне последний приобрел кинетическую энергию, равную его удвоенной энергии покоя. Под каким углом φ по отношению к направлению падающего фотона мог вылететь электрон?

О3.1-1.29

Фотон ($\lambda_0 = 662$ нм) рассеивается на электроне, летящем перпендикулярно направлению движения фотона. Найти начальный импульс электрона p_0, если длина волны λ_0 при рассеянии не изменяется. Угол рассеяния $\theta = 60°$.

О3.1-1.30 Угол разлета по потере энергии (!?!?)

Фотон с энергией $\mho_\gamma = 2m_ec^2$ (m_e - масса электрона) при рассеянии на покоящемся электроне теряет половину своей энергии. Найти угол разлета α между рассеянным фотоном и электроном отдачи.

Solution

(??? думаю, хорошая задача, но я слишком тупой для нее, основы не усвоены.)

О3.1-1.31 Рассеяние фотона на протоне

Фотон рассеивается на покоящемся протоне. Энергия рассеянного фотона равна кинетической энергии протона отдачи, а угол разлета между рассеянным фотоном и протоном отдачи равен 90°. Найти энергию $\mathcal{E}_\gamma$ падающего фотона.

Solution

О3.1-1.32 Сохранение энергии при рассеянии назад (!?!???!?)

С какой скоростью v должен двигаться электрон, чтобы летящий ему навстречу фотон с длиной волны $\lambda = 0,0024$ нм не изменил свою энергию при 180°-рассеянии?

Solution

Закон сохранения энергии с учетом релятивистской энергии электрона:

$$\hbar\omega + \frac{mc^2}{\sqrt{1+\beta^2}} = \hbar\omega + \frac{mc^2}{\sqrt{1+\beta'^2}}$$

Единственное решением это $\beta = \beta'$, то есть электрон летит назад с той же скоростью назад.

Закон сохранение импульса:

$$\frac{\hbar\omega}{c} - \frac{mc\beta}{\sqrt{1+\beta^2}} = -\frac{\hbar\omega}{c} + \frac{mc\beta}{\sqrt{1+\beta^2}}$$
$$\frac{mc\beta}{\sqrt{1+\beta^2}} = \frac{\hbar\omega}{c} = \frac{h}{\lambda}$$
$$\frac{\beta}{\sqrt{1+\beta^2}} = \frac{h}{mc}\frac{1}{\lambda} = \frac{\Lambda_c}{\lambda} \approx 1$$

Тут Λ_c - комптоновская длина, равная λ. Окончательно решаем уравнение на β и находим, что $v = c/\sqrt{2}$

О3.1-1.33

Оптический фотон с энергией $\hbar\omega_0$ рассеивается назад на электроне, движущемся ему навстречу с полной энергией $\mathscr{E}$ и импульсом p. Какова энергия рассеянного фотона? Рассмотреть два предельных случая:

а) $\frac{\mathscr{E}+pc}{mc^2} \cdot \frac{2\hbar\omega_0}{mc^2} \gg 1$;

б) $\frac{\mathcal{E}+pc}{mc^2} \cdot \frac{2\hbar\omega_0}{mc^2} \ll 1$.

Solution

О3.1-1.34

Определить энергию фотона hv', рассеянного назад покоящимся электроном. Какова эта энергия, если энергия падающего фотона hv удовлетворяет условию $hv \gg m_e c^2$ (m_e – масса электрона)?

Solution

О3.1-1.35 Обратный Комптон-эффект (!?!???!?!??)

Фотон от рубинового лазера ($\lambda = 0,6943$ мкм) испытывает лобовое соударение с электроном, имеющим кинетическую энергию $T = 500$ МэВ. Оценить энергию $\mathcal{E}_\gamma$ фотона, образующегося в результате «обратного комптон-эффекта» (т. е. при 180°-рассеянии фотона на движущемся электроне). См. также задачу 4.51 этого раздела.

Solution

Указание: рассмотреть два последовательных преобразования частоты из-за эффекта Доплера.

(??? подумаю про это, уже очень скоро!!!)

1.35. При условии $T \gg \hbar\omega_0$ ответ имеет вид $\mathscr{E}_\gamma \approx \hbar\omega_0 \frac{2T}{(m_e c^2)^2/(2T)+2\hbar\omega_0}$ (кинетическая энергия электрона $T \gg m_e c^2$, поэтому полная его энергия $\mathscr{E}_0 \approx T$). Здесь возможны два случая:

1) $\hbar\omega_0 \ll m_e c^2 \frac{m_e c^2}{T}$. Тогда $\mathscr{E}_\gamma \approx \hbar\omega_0 \left(\frac{2T}{m_e c^2}\right)^2 \approx 7,2$ МэВ (этот случай и реализуется в задаче).

2) $\hbar\omega_0 \gg m_e c^2 \frac{m_e c^2}{T}$. Тогда $\mathscr{E}_\gamma = \hbar\omega \approx T$. В задаче этот случай не выпол няется.

О3.1-1.36 Удваивание длины волны

Определить длину волны λ рентгеновского излучения, для которого комптоновское рассеяние на электроне на угол 90° удваивает длину волны.

Solution

(хз, с ходу совсем плохо это решаю.)
1.36. $\lambda = 2,4$ пм.

18.1.2 Problems about photons 2

О3.1-1.37

При движении быстрой заряженной частицы в области пространства, заполненной изотропным электромагнитным излучением (например, светом Солнца и звезд), частица теряет энергию в резуль тате взаимодействия с этим излучением. Считая частицу ультрарелятивистской (энергия $\mathscr{E}_0 \gg mc^2$), а ее соударения с фотоном - лобовыми, найти изменение энергии частицы $\Delta\tilde{\sigma} = \sigma_0 - \mathfrak{g}$ и энергию фотона отдачи $\hbar\omega$. Энергию фотонов (до соударения) $\hbar\omega_0$ считать малой по сравнению с $\hbar\omega$. Чему равна энергия $\hbar\omega$, если движущейся частицей является электрон с энергией $\mathscr{E}_0 = 2,5 \cdot 10^9$ эВ и $\hbar\omega_0 = 1$ эВ?

Solution

О3.1-1.38

Электрон с энергией $\mathscr{E}_0 \gg mc^2$ рассеивается на фотоне с энергией $\hbar\omega_0 \ll mc^2$. При каком условии энергия этого фотона в системе отсчета, в которой электрон покоится, удовлетворяет условию $\hbar\omega \ll mc^2$?

Solution

О3.1-1.39* Различение фотоэлектронов от комптоновских электронов (!!!!!!!!!!)

При прохождении γ-квантов через вещество образуются две группы быстрых электронов: одна в результате фотоэффекта, а другая - комптоновского рассеяния. Каково должно быть энергетическое разрешение регистрирующей аппаратуры, чтобы отличать фотоэлектроны от комптоновских электронов с максимальной энергией? Энергия γ-квантов известна: $\mathscr{E}_\gamma = 5$ МэВ.

Solution

(решена в задачнике. Очень нужно разобраться с этим, важная для понимания задача!!!!)

Ответ: $\frac{\Delta T}{T_\phi} = \left(1 + \frac{2\S}{m_e c^2}\right)^{-1} = 0,05$, где T_ϕ и $T_\text{К}$ - кинетические энергии электронов фотоэффекта и эффекта Комптона, $\Delta T = T_\phi - T_\text{К}$.

Р еш е н и е. Запишем закон Эйнштейна для фотоэффекта

$$h\nu = \mathscr{E}_{\text{ион}} + A + T_{\text{ф.}} .$$

где T_ϕ - кинетическая энергия фотоэлектрона, A - работа выхода вещества, $\mathcal{E}_{\text{ион}}$ - энергия ионизации электрона атома. Поскольку для самых глубоких K-электронов $\mathscr{E}_{\text{ион}} \leqslant 13,6 \cdot Z^2$ [эВ], где Z - заряд ядра, то даже для $Z \sim 10^2$ $\mathscr{E}_{\text{ион}} \lesseqgtr 0,136$ МэВ « $h\nu$. Величина работы выхода, как правило, не превышает 10 эВ, поэтому под действием γ-квантов (выокоэнергетичных фотонов) при фотоэффекте $T_\phi \simeq \mathscr{E}_\gamma$.

При Комптон-эффекте $\mathscr{E}_\gamma + m_e c^2 = \mathscr{E}'_\gamma + m_e c^2 + \mathscr{E}_{\text{ион}} + T_\text{К}$. Следовательно,

$$T_{\mathbf{k}} \approx \mathscr{E}_\gamma - \mathscr{E}'_\gamma = \frac{hc}{\lambda} - \frac{hc}{\lambda + \Delta\lambda} = \frac{hc}{\lambda}\frac{\Delta\lambda}{\lambda + \Delta\lambda}.$$

Энергия электрона в эффекте Комптона максимальна, когда фотон рассеивается назад, т. е.

$$\Delta\lambda = \Lambda_e(1 - \cos\varphi); \quad \Delta\lambda_{\max} = 2\Lambda_e = 2\frac{h}{m_e c}.$$

Таким образом,

$$T_\text{К} = \frac{hc}{\lambda}\frac{2h}{m_e c\lambda}\frac{1}{1 + \frac{2h}{m_e c\lambda}} = \mathscr{E}_\gamma \frac{2\mathscr{E}_\gamma}{m_e c^2}\frac{1}{1 + \frac{2E_\gamma}{m_e c^2}}.$$

Введем разрешение аппаратуры по энергии как $\Delta T = T_\phi - T_\text{к}$. Тогда

1.40 Анализ комптоновского рассеяния методом Брэгга-Вульфа

Фотоны с длиной волны $\lambda = 1,4$Å испытывают комптоновское рассеяние на угол $\varphi = 60^\circ$ к первоначальному направлению. Фотоны попадают в рентгеновский спектрограф, работающий по методу интерференционного отражения Брэгга-Вульфа. При какой минимальной толщине D кристаллической пластинки спектрографа можно обнаружить изменение длины волны рассеянного излучения (комптоновское смещение) в первом порядке, если постоянная кристаллической решетки $d = 1$Å?

Solution

Ответ: $D = \frac{\lambda d m_e c}{2\pi\hbar \sin^2(\varphi/2)} = 11,4$ нм.
Требуемая разрешающая способность спектрографа

$$R = \frac{\lambda}{\delta\lambda} = Nm$$

где N - число отражающих слоев, m - порядок интерференции. По формуле Брэгга-Вульфа $m = \frac{2d\sin\theta}{\lambda}$, где θ - угол скольжения; по условию $m = 1$, откуда

$$\sin\theta = \frac{\lambda}{2d}.$$

Изменение длины волны (комптоновское смещение)

$$\Delta\lambda = 2\pi A_e(1-\cos\varphi) = 4\pi \text{Å}_e \sin^2\frac{\varphi}{2}, \quad \text{где Å}_e = \frac{\hbar}{m_e c}3,86\cdot 10^{-11}\text{с}.$$

Таким образом,

$$R = Nm = \frac{D}{d}\frac{2d\cos\theta}{\lambda} = \frac{\lambda}{4\pi \text{Å}_e \sin^2(\varphi/2)}.$$

Отсюда

$$D = \frac{\lambda^2}{4\pi\hbar_e \sin^2(\varphi/2)\sin\theta} = \frac{\lambda d m_e c}{2\pi\hbar\sin^2(\varphi/2)} = 11,4\text{НМ}.$$

О3.1-1.41

Solution

(мб эта аналогичная, проверю потом)
$D_{\min} = \frac{\lambda^2}{4\Lambda_e \sin^2(\theta/2)\sin\varphi} = 2$НМ, $\Lambda_e = 0,0024$ - комптоновская длина волны электрона.

О3.1-1.42

Solution

Решение. Перейдем в систему центра масс пары. На пороге рождения скорость продуктов реакции равна нулю. Но γ-Квант и в этой системе движется со скоростью света, что противоречит закону сохранения импульса. Раз процесс невозможен в системе центра масс, то он невозможен и в других инерциальных системах, т.е. невозможен вообще.

О3.1-1.48. Нулевой сдвиг γ-кванта по энергии

Возбужденное ядро с энергией возбуждения $\Delta\mathscr{E} = 1$М и $A = 100$ движется с кинетической энергией $T = 100$ эВ и испускает гамма-квант. Под каким углом к направлению движения ядра сдвиг γ-кванта по энергии будет равен нулю?

Solution

Допплер уменьшает частоту, изменение скорости увеличивает частоту.
Эффекта Допплера:

$$\omega = \omega_0 \left(1 + \frac{v}{c}\cos\theta\right)$$

При излучении гамма-кванта скорость у ядра тоже меняется существенно. Импульсы ядра и гаммам-кванта в системе покоя ядра одинаковые и посчитаем это сдвиг частот:

$$\Delta\omega = \frac{T_{\text{new}}}{\hbar} = \frac{p^2}{2m\hbar} = \frac{E_\gamma}{2mc^2\hbar}$$
$$\omega = \frac{E_\gamma - T_{\text{new}}}{\hbar} = \frac{E_\gamma}{\hbar}\left(1 - \frac{E^\gamma}{2mc^2}\right)$$

С учетом этих двух сдвигов частот получаем:

$$\omega = \frac{E_\gamma}{\hbar}\left(1 + \frac{v}{c}\cos\theta - \frac{E_\gamma}{2mc^2}\right)$$

Вклады должны скомпенсировать друг друга:

$$\frac{v}{c}\cos\theta = \frac{E^\gamma}{2mc^2} \to \cos\theta = \frac{E_\gamma}{v - 2mc} = \frac{E_\gamma}{\sqrt{8Tmc^2}} \approx 0.116$$

(потом еще раз решу задачу!)

О3.1-1.49.

Рассматривая процесс рождения фотона с энергией $\hbar\omega$ при прохождении в веществе с показателем преломления n релятивистской частицы массой m со скоростью v (эффект Вавилова-Черенкова), показать, что обычно приводимое условие возможности этого процесса $v > v_\phi = c/n$ справедливо только при определенном ограничении на отношение A/λ (- комптоновская длина волны частицы, λ - длина волны фотона). Найти явное выражение этого ограничения в зависимости от релятивистского фактора γ и n.

О3.1-1.50.

По современным представлениям в спектре солнечных нейтрино должна существовать достаточно интенсивная монохроматическая линия с энергией $\mathscr{E}_v = 0,86\text{МВ}$, что обусловлено идущей на Солнце реакцией $^7\text{Be} + \text{e}^- \to {}^7\text{Li} + v_\text{e}$. Для регистрации этих нейтрино был создан детектор BOREXINO с жидким сцинтилятором, в котором регистрируются электроны по реакции рассеяния (ν, e^-). Какова максимальная кинетическая энергия регистрируемых электронов?

О3.1-1.52 высота полета спутника

В системе глобального позиционирования (GPS) используется высокоточный цезиевый генератор, установленный на спутнике. Определить высоту полета спутника, если при прохождении над приемником на Земле регистрируемая частота совпадает с частотой генератора. Учесть, что энергии квантовых уровней любой системы зависят от гравитационного потенциала в месте нахождения системы. Вращение Земли не учитывать. (См. также задачу 1.4 в этом разделе.)

Solution

1.52: $H = \frac{R_3}{2} \simeq 3200\text{КМ}$.
Решени е. Если считать Землю шаром, то гравитационный потенциал на поверхности Земли $\varphi_1 = -\gamma\frac{M}{R_3} = -v_1^2$, где v_1 - первая космическая скорость. На расстоянии r от центра Земли гравитационный потенциал $\varphi_2 = -\gamma\frac{M}{r}$. Фотон, испущенный на спутнике, имеет энергию

$$\hbar\omega_2 = \hbar\omega_0\sqrt{1 + 2\frac{\varphi_2}{c^2}} \approx \hbar\omega_0\left(1 + \frac{\varphi_2}{c^2}\right).$$

где ω_0 - частота генератора в нулевом поле. Из-за движения спутника (вслсдствие поперечного эффекта Доплера) на Земле этот сигнал будет иметь частоту

$$\omega_2' = \omega_2\sqrt{1 - \frac{v^2}{c^2}} \approx \omega_0\left(1 + \frac{\varphi_2}{c^2}\right)\left(1 - \frac{v^2}{2c^2}\right),$$

где $v = \sqrt{\gamma \frac{M}{r}}$ - скорость спутника. Расстояние между энергетическими уровнями приемника на Земле

$$\hbar\omega_1 = \hbar\omega_0 \sqrt{1 + 2\frac{\varphi}{c^2}} \approx \hbar\omega_0 \left(1 + \frac{\varphi_1}{c^2}\right).$$

Сдвига частоты не будет, если $\omega_1 = \omega_2'$, откуда

$$\frac{\varphi_2}{c^2} - \frac{v^2}{2c^2} = \frac{\varphi_1}{c^2} \text{ или } \frac{\varphi_2}{c^2} - \frac{\varphi_1}{c^2} = \frac{v^2}{2c^2}.$$

Подставляя значения, получим $-\gamma\frac{M}{r} + \gamma\frac{M}{R_3} = \gamma\frac{M}{2r}$, откуда $r = \frac{3}{2}R_3$.

(некоторые задачи не выгружал, ибо их слишком много)

1. Фотоны. Фотоэффект. Эффект Комптона SOLUTIONS

1.

13. $V_к = \frac{(2\pi\hbar c/\lambda) - A}{e} - V \approx -0,79$ В. Отрицательный знак означает, что при контакте цинка с материалом второго электрода фотоэлемента потенциал цинка окажется ниже.

1.

14. $\alpha = \sqrt{\frac{e}{WKt}} = 10^{-2}$, где e - заряд электрона.

1.

15. Решение. При «сухом» контакте потери на отражение от границы сцинтиллятор-фотокатод составляют несколько процентов, и ими можно пренебречь. Гораздо большую величину составляют потери на полное отражение при выходе из сцинтиллятора.

При «сухом» контакте на фотокатод попадают фотоны, идущие под углами $\theta_1 < \arcsin(1/n)$. Когда оптический контакт заполнен маслом - под углом $\theta_2 < \operatorname{arctg}(D/2h)$. Поскольку в сцинтилляторе фотоны испускаются изотропно, то отношение потоков равно

$$\frac{\Phi_2}{\Phi_1} = \frac{\int_0^{\theta_2} d\Omega}{\int_0^{\theta_1} d\Omega} = \frac{2\pi \int_0^{\theta_2} I_0 \sin\theta d\theta}{2\pi \int_0^{\theta_1} I_0 \sin\theta d\theta} = \frac{1 - \cos\theta_2}{1 - \cos\theta_1} \approx 3$$

1.

16. Решение. Рассмотрим сначала случай поглощения фотона нерелятивистским электроном. Выберем такую систему отсчета, в которой электрон сначала покоился. Законы сохранения энергии и импульса:

$$\hbar\omega = \frac{mv^2}{2}; \quad \frac{\hbar\omega}{c} = mv$$

Из написанных равенств следует $v = 2c$, что невозможно. Релятивисткое рассмотрение приводит к следующей системе уравнений:

$$\hbar\omega + mc^2 = \frac{mc^2}{\sqrt{1-\beta^2}}; \quad \frac{\hbar\omega}{c} = \frac{m\beta c}{\sqrt{1-\beta^2}}$$

откуда следует $\frac{1-\beta}{\sqrt{1-\beta^2}} = 1$, т. е. либо $\beta = 0$, либо $\beta = 1$. Первое условие означает, что поглощения не произошло, а второе - нереализуемо для массивной частицы. Таким образом показано, что свободный электрон не способен поглотить квант энергии. На частном случае показано, что трехчастичные реакции, т.е. реакции типа a + b $\leftrightarrows$ c невозможны (смотрите также задачу 8.13). Лишь при участиц в реакции четвертой частицы законы сохранения могут быть соблюдены.

Так как процессы поглощения и испускания обратимы по времени, то из невозможности прямого процесса следует невозможность обратного. Конечно, невозможность такого процесса можно показать и прямым вычислением, как это было сделано выше для случая поглощения.

1.

17. Длительность импульса определяется разбросом времени пролета электронов, вылетевших из фотокатода в направлении к аноду с различными направлениями начальной скорости, т. е. с величиной продольной составля-

ющей скорости от нуля до максимально возможной. Если обозначить времсна движения до анода t_1 и t_2, то

$$\Delta t = t_1 - t_2 = \frac{1}{eE}\sqrt{2mhc\left(\frac{1}{\lambda} - \frac{1}{\lambda_{\text{кр}}}\right)} = 1,2 \cdot 10^{-10}\text{с}.$$

1.

18. $t \geqslant 16\frac{A}{N}\frac{L^2}{d^2} = 455$ с, где N - мощность лампочки.

1.

19*. Решение. Пусть M - масса источника, а v - его скорость (рис. 135).

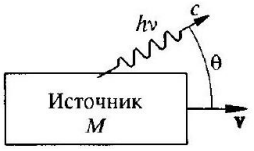


Рис. 135

Энергия источника слагается из кинетической энергии $Mu^2/2$ и внутренней энергии & возбужденных атомов. При испускании одного фотона внутренняя энергия $\mathscr{E}$ изменяется на вполне определенную величину (энергия квантуется!) $\mathscr{E} - \mathscr{E}' = hv_0$, где v_0 - частота фотона, испускаемого неподвижным источником. При испускании фотона тело испытывает отдачу, и его скорость меняется. По закону сохранения энергии

$$\frac{1}{2}Mv^2 + \mathscr{E} = \frac{1}{2}Mv'^2 + \mathscr{E}' + hv$$

где v - частота фотона, излучаемого движущимся источником. Написав закон сохранения импульса и спроектировав его на направление скорости $\mathbf{v}$ и на перпендикулярное направление, получим

$$Mv = Mv'\cos\alpha + \frac{hv}{c}\cos\theta, \quad 0 = Mv'\sin\alpha - \frac{hv}{c}\sin\theta$$

где θ и α - углы между направлением скорости v и направлениями импульсов испущенного фотона и источника после испускания. Исключая v' и α, найдем

$$2Mh\,(v - v_0) - 2Mv\frac{hv}{c}\cos\theta + \frac{h^2v^2}{c^2} = 0$$

Если масса источника M достаточно велика, то можно пренебречь последним членом, и мы получим, учитывая, что по условию $v/c \ll 1$,

$$v = \frac{v_0}{1 - \frac{v}{c}\cos\theta} \simeq v_0\left(1 + \frac{v}{c}\cos\theta\right)$$

1.

20*. Решение. Пусть $\mathscr{E}$ и $\mathscr{E}'$ - полные энергии тела до и после излучения. Соответственно $\mathscr{E}_0$ и $\mathscr{E}_0$ - энергия покоя, а p и p ′ - импульсы. Обозначим также энергию и импульс излученного фотона как ε и $\mathbf{q}$ и запишем законы сохранения

$$\mathscr{E}' = \mathscr{E} - \varepsilon; \quad \mathbf{p} = \mathbf{p}' + \mathbf{q}.$$

Возведем эти уравнения в квадрат и вычтем, предварительно домножив второе соотношение на c^2. Учитывая, что $\varepsilon = qc$, а $\mathscr{E}^2 - p^2c^2 = \mathscr{E}_0^2$ и $\mathscr{E}'^2 - p'^2c^2 = \mathscr{E}_0'^2$, получим

$$\mathscr{E}_0'^2 = \mathscr{E}_0^2 - 2\mathscr{E}\varepsilon + 2c^2pq$$

Релятивистский импульс тела $p = \&\beta/c$, где $\beta = v/c$. Подставляя это в полученное уравнение, находим

$$\mathscr{E}_0 - \mathscr{E}_0' = \frac{2\mathscr{E}}{\mathscr{E}_0 + \mathscr{E}_0'}\varepsilon(1 - \beta\cos\theta),$$

где θ - угол между импульсом тела $\mathbf{p}$ и направлением вылета фотона (рис. 135).
Для массивного тела $Mc^2 \gg h\nu$, откуда $\mathscr{E}_0' \approx \mathscr{E}_0$, и тогда

$$\mathscr{E}_0 - \mathscr{E}_0' \approx \frac{\mathscr{E}}{\mathscr{E}_0}\varepsilon(1 - \beta\cos\theta), \text{ или } (\mathscr{E}_0 - \mathscr{E}_0')\sqrt{1-\beta^2} = \varepsilon(1 - \beta\cos\theta).$$

Поскольку $\mathscr{E}_0 - \mathscr{E}_0' = h\nu$, а $\varepsilon = h\nu'$, то получим искомую связь частот неподвижного и движущегося источников

$$v' = v\frac{\sqrt{1-\beta^2}}{1 - \beta\cos\theta}.$$

При $\theta = \frac{\pi}{2}$ смещение частоты $\Delta v = v_0\frac{v^2}{2c^2}$, а при $\beta \ll 1$ принимаемая частота $\nu \approx \nu_0\left(1 + \frac{v}{c}\cos\theta\right)$ и $\Delta v = \frac{v}{c}\cos\theta$.

1.

21: Решение. При $\theta = 0 \quad \nu(0) = v_0\frac{\sqrt{1-\beta^2}}{1-\beta}$. При $\theta = \frac{\pi}{2}$ эта частота $v(\pi/2) = v_0\sqrt{1-\beta^2}$. Если $\beta \to 1$, то $v(0) \gg v(\pi/2)$. Отсюда ясно, что в узкой окрестности угла $\theta = 0$ частоты излучаемого света особенно велики. Найдем угол θ, для которого $v(\theta) = \alpha\nu(0)$, где $\alpha < 1$. Для этого угла нетрудно получить

$$\cos\theta \approx 1 - \frac{\theta^2}{2} = \frac{1 - (1-\beta)/\alpha}{1 - (1-\beta)} \approx 1 - \frac{1-\alpha}{\alpha}(1-\beta)$$

откуда

$$\theta^2 = 2\frac{1-\alpha}{\alpha}(1-\beta).$$

Так как $\sqrt{1-\beta^2} = mc^2/\mathscr{E}$, где $\mathscr{E}$ - полная энергия частицы, то $1 - \beta \approx \frac{1}{2}\left(\frac{mc^2}{\varrho}\right)^2$. Это дает

$$\theta = \sqrt{\frac{1-\alpha}{\alpha}}\frac{mc^2}{\varrho}.$$

При $\alpha = 1/2$ получаем $\theta = mc^2/\mathscr{E}$, иначе говоря, частота излучения падает вдвое под углом $\theta = mc^2/\mathscr{E} = \sqrt{1-\beta^2} = \gamma^{-1}$.

1.

22. $\Delta\lambda = \Lambda_e(1 - \cos\theta) = \lambda_1 - \lambda_0 = \lambda_0 = 4 \cdot 10^{-3}$ нм.

1.

23. $T_e = \frac{2hc}{\lambda}\frac{\Lambda_e \sin^2(\theta/2)}{\lambda + 2\Lambda_e \sin^2(\theta/2)}, (p_e c)^2 = T_e^2 + 2m_e c^2 T_e$.
Здесь $\Lambda_e = 2,4263 \cdot 10^{-3}$ нм - комптоновская длина волны электрона. При $\theta = 90°$

$$T_e = \frac{hc}{\lambda}\frac{\Lambda_e}{\lambda + \Lambda_e} = 0,108\frac{hc}{\lambda} = 0,67 \cdot 10^4\rho\text{В}, \quad cp_e = 8,3 \cdot 10^4\rho \text{ В},$$

т. е. фотон передал электрону около 10% своей энергии, а импульс электрона отдачи по абсолютной величине оказался больше импульса первичного фотона.

1.

24. Решение. Как видно из рис. 136 , из закона сохранения импульса следует
$p_e \cos\varphi = \frac{h\nu}{c} - \frac{h\nu'}{c}\cos\theta, \quad p_e \sin\varphi = \frac{h\nu'}{c}\sin\theta.$
Почленным делением находим

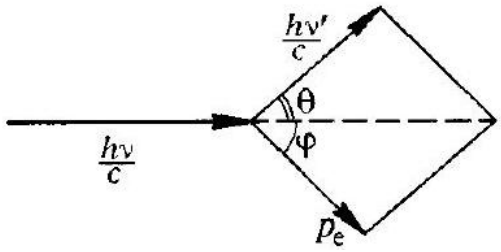


Рис. 136

$$\operatorname{tg}\varphi = \frac{\sin\theta}{\nu/\nu - \cos\theta}$$

Отсюда с учетом соотношения $\frac{v}{v'} - 1 = \frac{2h\nu}{m_e c^2}\sin^2\theta$ легко получить

$$\operatorname{tg}\varphi = \frac{\operatorname{ctg}(\theta/2)}{1 + \frac{h\nu}{m_e c^2}}.$$

При $\theta = 90^\circ$ $\operatorname{tg}\varphi = 0,8916, \varphi = 41^\circ 43'$.

1.

25. $\Delta\lambda = \frac{2h}{m_e c}\sin^2\frac{\theta}{2} = \frac{h}{m_e c} = 2,4263 \cdot 10^{-3}$НМ.

1.

26. $0 \leqslant \varphi < \arccos\left(\sqrt{1 + \left(\frac{mc}{p}\right)^2} - \frac{mc}{p}\right)$.

Решение. Запишем закон сохранения импульса в соответствии с рис. 2: $\mathbf{p}'_\gamma = \mathbf{p}_\gamma - \mathbf{p}$, откуда по теореме косинусов

$$\left(\frac{h\nu'}{c}\right)^2 = \left(\frac{h\nu}{c}\right)^2 - \frac{2h\nu}{c}p\cos\varphi + p^2.$$

Закон сохранения энергии:

$$\mathfrak{E}'_\gamma = \mathscr{E}_\gamma - T = \mathscr{E}_\gamma - \mathscr{E} + mc^2, \text{ т. е.}$$
$$h\nu' = h\nu - \sqrt{(pc)^2 + (mc^2)^2} + mc^2$$

Исключая $h\nu'$, получим

$$h\nu = \frac{(pc)^2 - T^2}{2(pc\cos\varphi - T)}.$$

Определим знак числителя:

$$\begin{aligned}&(pc)^2 - T^2 = \\ &= (pc)^2 - \left[(pc)^2 + \left(mc^2\right)^2 - 2\sqrt{(pc)^2 + (mc^2)^2}\cdot mc^2 + \left(mc^2\right)^2\right] = \\ &= 2mc^2\left(\sqrt{(pc)^2 + (mc^2)^2} - mc^2\right) > 0\end{aligned}$$

всегда. Так как $h\nu > 0$, то и знаменатель полученной дроби тоже положителен: $pc\cos\varphi - T > 0$, откуда $\cos\varphi > \frac{T}{pc} = \sqrt{1 + \left(\frac{mc}{p}\right)^2} - \frac{mc}{p}$. Таким обра-
зом, диапазон углов, под которым мог вылететь электрон с заданным имнульсом, лежит в пределах

$$0 \leqslant \varphi < \arccos\left(\sqrt{1+\frac{m^2c^4}{p^2}}-\frac{mc}{p}\right).$$

1.

27. $T < 2mc^2 \operatorname{ctg}^2\varphi = 0,34$М В В.

1.

28. $0 \leqslant \varphi < 45°$.

1.

29. $p_0 = \frac{2\pi\hbar}{\lambda_0}\operatorname{tg}\frac{\theta}{2} \approx 6\cdot 10^{-23}$Г $\cdot$ см/с.

1.

30. $\alpha = 90°$.

1.

31. $\mathscr{E}_\gamma = 2m_\text{p}c^2 \approx 1,9$ ГэВ, где m_p - масса протона.

1.

32. $v = \frac{c}{\sqrt{1+\lambda/\Lambda_e}} \approx \frac{c}{\sqrt{2}}$, где $\Lambda_\text{e} = \frac{h}{mc} = 0,0024$ нм - комптоновская длина волны электрона.

1.

33. $\hbar\omega' = \hbar\omega_0 \frac{\left(\frac{8+pc}{mc^2}\right)^2}{1+\frac{2\hbar\omega_0}{mc^2}\frac{8+pc}{mc^2}}$, где p - импульс электрона.

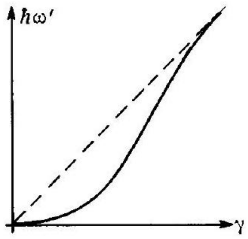


Рис. 137

Случай а) $\hbar\omega' = \frac{\varrho + pc}{2} \approx \mathscr{E}$

Ультрарелятивистский электрон ($\mathfrak{E} \approx pc$) передает фотону всю свою энергию (пунктир на рис. 137).
Случай б) $\hbar\omega' = \hbar\omega_0\left(\frac{\mathscr{E}+pc}{mc^2}\right)^2 \approx 4\gamma^2\hbar\omega_0$, где $\gamma = \frac{1}{\sqrt{1-v^2/c^2}}$.
Таким образом, в этом случае $\hbar\omega' \propto \gamma^2$ (рис. 137).

1.

34.

$$hv' = \frac{hv}{1+\frac{2hv}{m_e c^2}}. \quad \text{Если} \quad hv \gg m_e c^2, \quad \text{то}$$

$hv' \approx m_e c^{2/2}$.

1.

35. При условии $T \gg \hbar\omega_0$ ответ имеет вид $\mathscr{E}_\gamma \approx \hbar\omega_0 \frac{2T}{(m_e c^2)^2/(2T)+2\hbar\omega_0}$ (кинетическая энергия электрона $T \gg m_e c^2$, поэтому полная его энергия $\mathfrak{E}_0 \approx T$). Здесь возможны два случая:

1. $\hbar\omega_0 \ll m_e c^2 \frac{m_e c^2}{T}$. Тогда $\wp_\gamma \approx \hbar\omega_0 \left(\frac{2T}{m_e c^2}\right)^2 \approx 7,2$ МэВ (этот случай и реализуется в задаче).

2. $\hbar\omega_0 \gg m_e c^2 \frac{m_e c^2}{T}$. Тогда $\mathscr{E}_\gamma = \hbar\omega \approx T$. В задаче этот случай не выполь няется.

Указание: рассмотреть два последовательных преобразования частоты из-за эффекта Доплера.

1.

36. $\lambda = 2,4$ пм.

1.

37. $\Delta\delta = \hbar\omega = \left(\frac{2\mathscr{E}}{mc^2}\right)^2 \frac{\hbar\omega_0}{1+4\varrho\hbar\omega_0/(m^2c^4)}$.

Если $\mathscr{E}_0 \ll mc^2\left(mc^2/4\hbar\omega_0\right)$, то $\hbar\omega \approx \left(2\mathscr{E}/mc^2\right)^2 \hbar\omega_0 \ll \mathscr{E}_0$. В противоположном предельном случае $\hbar\omega \approx \mathscr{E}_0$. В приведенном примере $\hbar\omega = 10^8$ эВ.

1.

38. По формуле для эффекта Доплера

$$\omega_0 = \frac{\omega\sqrt{1-v^2/c^2}}{1+v/c}$$

(фотон и электрон считаются движущимися навстречу друг другу, причем скорость электрона равна v). В ультрарелятивистском случае отсюда следует, что $\omega_0 = \omega mc^2/2\varrho_0$, и условие $\hbar\omega \ll mc^2$ принимает вид

$$\mathscr{E}_0 \ll \frac{\left(mc^2\right)^2}{2\hbar\omega_0}$$

1.

39: $\frac{\Delta T}{T_\phi} = \left(1+\frac{2\mathscr{E}}{m_e c^2}\right)^{-1} = 0,05$, где $T_\text{ф}$ и $T_\text{к}$ - кинетические энергии электронов фотоэффекта и эффекта Комптона, $\Delta T = T_\phi - T_\text{к}$.

Решение. Запишем закон Эйнштейна для фотоэффекта

$$hv = \mathfrak{E}_\text{ион} + A + T_\text{ф}$$

где T_ϕ - кинетическая энергия фотоэлектрона, A - работа выхода вещества, $\mathscr{E}_\text{ион}$ - энергия ионизации электрона атома. Поскольку для самых глубоких K-электронов $\mathscr{E}_\text{ион} \leqslant 13,6 \cdot Z^2$[], где Z - заряд ядра, то даже для $Z \sim 10^2$ $\mathscr{E}_\text{ион} \leq 0,136$М ВВ $\ll hv$. Величина работы выхода, как правило, не превышает 10 эВ,

поэтому под действием γ-квантов (выокоэнергетичных фотонов) при фотоэффекте $T_\phi \simeq \mathscr{E}_\gamma$.
При Комптон-эффекте $\mathscr{E}_\gamma + m_\mathrm{e}c^2 = \mathfrak{E}'_\gamma + m_\mathrm{e}c^2 + \mathscr{E}_{\text{ион}} + T_\text{к}$. Следовательно,

$$T_\mathbf{K} \approx \mathscr{E}_\gamma - \mathscr{E}'_\gamma = \frac{hc}{\lambda} - \frac{hc}{\lambda + \Delta\lambda} = \frac{hc}{\lambda}\frac{\Delta\lambda}{\lambda + \Delta\lambda}$$

Энергия электрона в эффекте Комптона максимальна, когда фотон рассеивается назад, т. е.

$$\Delta\lambda = \Lambda_\mathrm{e}(1 - \cos\varphi); \quad \Delta\lambda_\text{max} = 2\Lambda_\mathrm{e} = 2\frac{h}{m_\mathrm{e}c}$$

Таким образом,

$$T_\mathrm{K} = \frac{hc}{\lambda}\frac{2h}{m_\mathrm{e}c\lambda}\frac{1}{1 + \frac{2h}{m_\mathrm{e}c\lambda}} = \mathscr{E}_\gamma\frac{2\mathscr{E}_\gamma}{m_\mathrm{e}c^2}\frac{1}{1 + \frac{2\delta_\gamma}{m_\mathrm{e}c^2}}$$

Введем разрешение аппаратуры по энергии как $\Delta T = T_\Phi - T_\mathrm{k}$. Тогда

$$\frac{\Delta T}{T_\phi} \approx \frac{\varrho_\gamma - T_\mathrm{K}}{\varrho_\gamma} = \frac{1}{1 + \frac{\delta_\gamma}{m_\mathrm{e}c^2}} \simeq 0,05(5\%)$$

1.

40* $D = \frac{\lambda d m_\mathrm{e} c}{2\pi\hbar\sin^2(\varphi/2)} = 11,4\text{НМ}$.
Репение. Требуемая разрешающая способность спектрографа

$$R = \frac{\lambda}{\delta\lambda} = Nm$$

где N - число отражающих слоев, m - порядок интерференции. По формуле Брэгга-Вульфа $m = \frac{2d\sin\theta}{\lambda}$, где θ - угол скольжения; по условию $m = 1$, откуда

$$\sin\theta = \frac{\lambda}{2d}.$$

Изменение длины волны (комптоновское смещение)

$$\Delta\lambda = 2\pi\text{Å}_\mathrm{e}(1 - \cos\varphi) = 4\pi\text{Å}_\mathrm{e}\sin^2\frac{\varphi}{2}, \text{ где } \mathrm{A_e} = \frac{\hbar}{m_\mathrm{e}c}3,86\cdot10^{-11}\text{ cm}.$$

Таким образом,

$$R = Nm = \frac{D}{d}\frac{2d\cos\theta}{\lambda} = \frac{\lambda}{4\pi\star_\mathrm{e}\sin^2(\varphi/2)}.$$

Отсюда

$$D = \frac{\lambda^2}{4\pi\hbar_\mathrm{e}\sin^2(\varphi/2)\sin\theta} = \frac{\lambda d m_\mathrm{e} c}{2\pi\hbar\sin^2(\varphi/2)} = 11,4\text{НМ}.$$

1.

41. $D_\text{min} = \frac{\lambda^2}{4\Lambda_e\sin^2(\theta/2)\sin\varphi} = 2\text{НМ}, \Lambda_\mathrm{e} = 0,0024$ нм - комптоновская длина волны электрона.

1.

42: Решение. Перейдем в систему центра масс пары. На пороге рождения скорость продуктов реакции равна нулю. Но γ-квант и в этой системе движется со скоростью света, что противоречит закону сохранения импульса. Раз процесс невозможен в системе центра масс, то он невозможен и в других инерциальных системах, т. е. невозможен вообще.

1.

44. $\theta_\text{max} = 60°$.

1.

45. $\theta_{12} = 90°; \theta_{13} = \pi - \operatorname{arctg}\frac{4}{3} \approx 127°; \theta_{23} = \pi - \operatorname{arctg}\frac{3}{4} \approx 143°$.

1.

46. $\mathscr{E}_1 = 0,85\mathscr{E}_0 = 432$ кэВ; $\mathscr{E}_2 = \frac{2}{3+\sqrt{3}}\mathscr{E}_0 \approx 216$ кэВ; $\mathscr{E}_3 = \sqrt{3}\mathscr{E}_2 \approx \approx 374$ кэВ.

1.

47. Решение. Преобразование Лоренца для энергии частицы $\mathscr{E}$, импульс которой p,

$$\mathscr{E}' = \frac{\mathscr{E} - vp\cos\theta}{\sqrt{1 - v^2/c^2}}$$

где v - скорость штрихованной (движущейся) системы отсчета, а θ - угол в неподвижной системе между направлением движения фотона и скоростью источника. Энергия фотона $\mathscr{E} = h\nu = pc$, тогда

$$\nu' = \nu\frac{1 - (v/c)\cos\theta}{\sqrt{1 - v^2/c^2}}$$

Здесь ν - частота света в неподвижной системе отсчета, ν' - в движущейся вместе с источником. Переписывая ее в общепринятом виде, получим

$$\nu = \nu'\frac{\sqrt{1 - v^2/c^2}}{1 - (v/c)\cos\theta}$$

1.

48. $\cos\theta = \frac{\Delta\mathscr{E}}{2\sqrt{2Tm_{\text{яд}}\,c^2}} = 0,116, \theta = 83,3°$; где $m_{\text{яд}}\,c^2 = A \cdot 931,5$М ВВ.

1.

49. $\frac{\text{Å}}{\lambda} \leqslant \left(\frac{n\nu}{c} - 1\right)\frac{2\gamma}{n^2-1} < \frac{2\gamma}{n^2-1}$.

1.

50. $T_{\text{e}}^{\max} = \mathscr{E}_\nu\frac{\Delta\lambda^{\max}}{\lambda+\Delta\lambda^{\max}} = 663$ кэВ, где $\Delta\lambda^{\max} = \lambda' - \lambda = 2\Lambda_{\text{e}}$; $\lambda = \frac{hc}{\mathscr{E}_\nu}$ (комптон-эффект нейтрино на электронах).

1.

51: Длина волны гамма-квантов от источника равна $\lambda = 1,88\cdot10^{-10}$ см $\gg R_{\text{яд}}$, поэтому комптоновское рассеяние идет не на нуклонах ядра, а на ядре в целом (но не на молекуле, т.к. $\lambda \ll R_{\text{мол}} \simeq 3$Å для H_2O). Комптон-эффект на протоне $\Delta\lambda_{\text{H}}$ отличается от соответствующего эффекта на дейтроне $\Delta\lambda_{\text{D}}$. Таким образом,

$$\left|\frac{\Delta\varrho}{\varrho}\right| = \frac{|\Delta\lambda_{\text{H}} - \Delta\lambda_{\text{D}}|}{\lambda} = \frac{\varrho}{2m_{\text{p}}c^2} = 3,6\cdot10^{-4}$$

1.

52* $H = \frac{R_3}{2} \simeq 3200$ км.

Решение. Если считать Землю шаром, то гравитационный потенциал на поверхности Земли $\varphi_1 = -\gamma\frac{M}{R_3} = -v_1^2$, где v_1 - первая космическая скорость. На расстоянии r от центра Земли гравитационный потенциал $\varphi_2 = -\gamma\frac{M}{r}$.

Фотон, испущенный на спутнике, имеет энергию

$$\hbar\omega_2 = \hbar\omega_0\sqrt{1+2\frac{\varphi_2}{c^2}} \approx \hbar\omega_0\left(1+\frac{\varphi_2}{c^2}\right)$$

где ω_0 - частота генератора в нулевом поле.

Из-за движения спутника (вследствие поперечного эффекта Доплера) на Земле этот сигнал будет иметь частоту

$$\omega_2' = \omega_2\sqrt{1-\frac{v^2}{c^2}} \approx \omega_0\left(1+\frac{\varphi_2}{c^2}\right)\left(1-\frac{v^2}{2c^2}\right)$$

где $v = \sqrt{\gamma\frac{M}{r}}$ - скорость спутника. Расстояние между энергетическими уровнями приемника на Земле

$$\hbar\omega_1 = \hbar\omega_0\sqrt{1+2\frac{\varphi}{c^2}} \approx \hbar\omega_0\left(1+\frac{\varphi_1}{c^2}\right)$$

Сдвига частоты не будет, если $\omega_1 = \omega_2'$, откуда

$$\frac{\varphi_2}{c^2} - \frac{v^2}{2c^2} = \frac{\varphi_1}{c^2} \text{ или } \frac{\varphi_2}{c^2} - \frac{\varphi_1}{c^2} = \frac{v^2}{2c^2}$$

Подставляя значения, получим $-\gamma\frac{M}{r} + \gamma\frac{M}{R_3} = \gamma\frac{M}{2r}$, откуда $r = \frac{3}{2}R_3$.

18.1.3 Problems about Special Effects in Atoms 1

Б-2.11.1 Конечное ядро водорода

Найти смещение уровня энергии основного состояния атома водорода под влиянием конечных размеров ядра. Ядро считать равномерно заряженным по объему шаром радиуса r_0.

Solution

Считаем поправку по теории возмущений, нужно знать поле от равномерно заряженного шара, что считается элементарными методами электродинамики.

$$H \equiv H_0 + V = \frac{\mathbf{p}^2}{2m} - \frac{e^2}{r} + V(r).$$

$$V(r) \equiv U(r) - \left(-\frac{e^2}{r}\right)$$

$$\psi_{(0)}(\mathbf{r}) = \langle\mathbf{r}|\psi_{(0)}\rangle = R_{10}(r)\cdot Y_{00}(\vartheta,\varphi) = \frac{1}{\sqrt{\pi a^3}}e^{-\frac{r}{a}}.$$

Найдем поправку по теории возмущений. Сперва определим потенциал внутри равномерно заряженного шара.

$$q = e\frac{r^3}{R^3} \qquad \mathcal{E}(r) = e\frac{r}{R^3}, \qquad U(r) = e\int\mathcal{E}(r)dr + c_0 = e^2\frac{r^2}{2R^3} + c_0$$

$U(r)|_{r=R} = -\frac{e^2}{R}$, поэтому $c_0 = -\frac{3e^2}{2R}$. В итоге

$$U(r) = \begin{cases} \dfrac{e^2r^2}{2R^3} - \dfrac{3e^2}{2R}, & r \le R \\ -\dfrac{e^2}{r}, & r \ge R \end{cases}$$

. Поправка к энергии ϵ_1 в первом порядке теории возмущений равна:

$$\epsilon_1 = \langle\psi_{(0)}|V|\psi_{(0)}\rangle = 4\pi\int\limits_0^R dr\frac{r^2}{\pi a^3}\left(\frac{e^2r^2}{2R^3} - \frac{3e^2}{2R} + \frac{e^2}{r}\right)e^{-\frac{2r}{a}} \overset{R\ll a}{\approx}$$

$$\overset{\exp\approx 1}{\approx} = \frac{4}{a^3}\int\limits_0^R dr\left(\frac{e^2r^4}{2R^3} - \frac{3e^2r^2}{2R} + e^2r\right) = \frac{4}{a^3}\frac{e^2R^2}{10} = \frac{2}{5}\frac{e^2R^2}{a^3}$$

Б-2.11.2 Поляризуемость водорода в основном состоянии

Вычислить электрическую поляризуемость атома водорода, находящегося в основном состоянии. Показать, что для нахождения поляризуемости атома, находящегося в основном состоянии, достаточно знать лишь поправку второго порядка $E^{(2)}$.

Solution

Используем обычную теорию возмущений.
Атом водорода в поле $\mathcal{E} = \{0, 0, \mathcal{E}\}$, в атомной системе единиц $h = m = e = 1$ имеет

$$\hat{\mathrm{H}} = \frac{\hat{\mathrm{p}}^2}{2} - \frac{1}{r} + \mathcal{E}r\cos\theta \equiv \hat{\mathrm{H}}^{(0)} + \hat{\mathrm{V}},$$

Здесь $\mathcal{E}$ есть отношение напряженности внешнего электрического поля к внутриатомному $\varepsilon_a = e/a^2 \simeq 5,14\cdot 10^9$ В/см, поэтому практически всегда $\mathcal{E} \ll 1$, т. е. можно использовать теорию возмущений.

В основном состоянии у электрона $\psi^{(0)}(r) = \psi_{100} = \frac{1}{\sqrt{\pi}}e^{-r}$, поэтому поправка первого приближения к энергии $E_0^{(1)} = \langle\psi^{(0)}|\hat{V}|\psi^{(0)}\rangle = 0$ в силу сферической симметрии основного состояния и.

Во втором порядке теории возмущений

$$E_0^{(2)} = -\frac{1}{2}\alpha\mathcal{E}^2,$$

где $\alpha = -\frac{\partial^2 E_0^{(2)}}{\partial\mathcal{E}^2}$- поляризуемость атома.

$$E_0^{(2)} = \langle\psi^{(1)}|\hat{\mathbf{V}}|\psi^{(0)}\rangle = \int\psi^{(1)}(\mathbf{r})\mathcal{E}r\cos\theta\psi^{(0)}(\mathbf{r})d^3x,$$

где поправка первого приближения $\psi^{(1)}$ удовлетворяет уравнению первого приближения теории возмущений:

$$\left(\hat{\mathrm{H}}^{(0)} - E^{(0)}\right)\psi^{(1)}(\mathbf{r}) = -\hat{\mathrm{V}}\psi^{(0)}(\mathbf{r}), \qquad E^{(0)} = -\frac{1}{2},$$

$$\left(-\frac{1}{2}\Delta - \frac{1}{r} + \frac{1}{2}\right)\psi^{(1)}(\mathbf{r}) = -\frac{\varepsilon r\cos\theta}{\sqrt{\pi}}e^{-r} = -\frac{2}{\sqrt{3}}\mathcal{E}re^{-r}Y_1^{(0)}(\theta,\varphi).$$

где $Y_1^{(0)}(\theta,\varphi) = \sqrt{3/4\pi}\cos\theta$.

Подставим анзац $\psi^{(1)}(\mathbf{r}) = f(r)e^{-r}Y_1^{(0)}(\theta,\varphi)$, где $f(r) = a+br+cr^2$, определим коэффициенты, находим окончательно

$$\psi^{(1)}(\mathbf{r}) = -\frac{2\mathcal{E}}{\sqrt{3}}r\left(1+\frac{r}{2}\right)e^{-r}Y_1^{(0)}(\theta,\varphi).$$

В итоге

$$E_0^{(2)} = -\int\frac{2\mathcal{E}}{\sqrt{3}}r\left(1+\frac{r}{2}\right)e^{-r}Y_1^{(0)}(\theta,\varphi)\mathcal{E}r\cos\theta\frac{1}{\sqrt{\pi}}e^{-r}d^3x = -\frac{4}{3}\varepsilon^2\int\limits_0^\infty r^4\left(1+\frac{r}{2}\right)e^{-2r}dr = -\frac{9}{4}\varepsilon^2.$$

Поэтому $\alpha = 9/2$, а в обычной системе единиц

$$\alpha = (9/2)a^3.$$

Б-2.11.3 Эффект Штарка

Найти расщепление в однородном электрическом поле уровня энергии атома водорода с $n = 2$ (эффект Штарка). Найти правильные волновые функции нулевого приближения.

Solution

Решаем обычной теории возмущений для вырожденных уровней.
Атом водорода в поле $\mathcal{E} = \{0, 0, \mathcal{E}\}$, в атомной системе единиц $h = m = e = 1$ имеет

$$\hat{\mathrm{H}} = \frac{\hat{\mathrm{p}}^2}{2} - \frac{1}{r} + \mathcal{E}r\cos\theta \equiv \hat{\mathrm{H}}^{(0)} + \hat{\mathrm{V}},$$

В случае $n = 2$ энергетические поправки оказываются пропорциональны первой степени $\mathcal{E}$ - имеет место линейный эффект Штарка. Причиной этого является случайное вырождение уровней энергии, благодаря которому возбужденные состояния не обладают определенной четностью, и у атома появляется отличный от нуля средний дипольный электрический момент.

Для невозмущенной задачи $E_2^{(0)} = -Z^2/8$, и кратность вырождения $n^2 = 4$, поэтому необходимо применять теорию возмущений для вырожденных уровней энергий. Уровню $E_2^{(0)}$ отвечают четыре собственные функции:

$$\psi_{200} = R_{20}(r)Y_0^{(0)}(\theta,\varphi), \qquad \psi_{210} = R_{21}(r)Y_1^{(0)}(\theta,\varphi), \qquad \psi_{21\pm1} = R_{21}(r)Y_1^{(\pm1)}(\theta,\varphi),$$

где

$$R_{20}(r) = \left(\frac{Z}{2}\right)^{3/2} e^{-\frac{Zr}{2}} 2\left(1 - \frac{Zr}{2}\right), \qquad R_{21}(r) = \left(\frac{Z}{2}\right)^{3/2} e^{-\frac{Zr}{2}\frac{Zr}{\sqrt{3}}},$$

Считаем матричные элементы оператора возмущений. Вычисления показывают, что отличны от нуля лишь следующие:

$$\langle\psi_{200}|\hat{\mathrm{V}}|\psi_{210}\rangle = \langle\psi_{210}|\hat{\mathrm{V}}|\psi_{200}\rangle = -3\frac{\varepsilon}{Z}.$$

Решая секулярное уравнение, получаем поправки к уровню энергии $E_2^{(0)}$:

$$E_{1,4}^{(1)} = \mp 3\frac{\varepsilon}{Z}, \qquad E_{2,3}^{(1)} = 0.$$

Таким образом, исходный уровень энергии $E_2^{(0)}$ под действием электрического поля расщепляется на три уровня с энергиями:

$$E_{1,3} = E_2^{(0)} \pm E_{1,4}^{(1)} = E_2^{(0)} \mp 3\frac{\varepsilon}{Z}, \qquad E_2 = E_2^{(0)}.$$

Уровню энергии E_1 отвечает правильная функция нулевого приближения $\phi_1 = \frac{1}{\sqrt{2}}(\psi_{200} + \psi_{210})$, уровню E_3 соответствует состояние $\phi_4 = \frac{1}{\sqrt{2}}(\psi_{200} - \psi_{210})$, а уровень E_2 двукратно вырожден ему отвечают две линейно независимые функции: ψ_{211} и ψ_{21-1}.

Б-2.11.4 Сверхтонкое расщепление основного состояния водорода

Найти величину сверхтонкого расщепления основного состояния атома водорода.
Напоминание: по определению, под сверхтонким расщеплением имеется в виду изменение энергии при учете взаимодействия между ядром и электроном.

Solution

Считаем добавку к энергии за счет поля от магнитного момента протона методами теории поля, далее по теории возмущений получаем расщепление уровней энергии.
(??? почему квадрупольное вз-е не учитываем тут???)

Ядро атома водорода (протон) обладает собственным магнитным моментом μ_p. Взаимодействие магнитного момента электрона с магнитным полем ядра приводит к расщеплению атомных уровней по значению полного углового момента атома. Поскольку значение ядерного магнитного момента примерно в 10^3 раз меньше, чем значение орбитального магнитного момента электрона, то и соответствующее расщепление примерно в 10^3 раз меньше, чем расщепление тонкой структуры. Поэтому такое расщепление называют сверхтонким расщеплением. Гамильтониан сверхтонкого взаимодействия имеет вид

$$\hat{\mathrm{V}}^{\text{hyp-f}} = -\left(\hat{\mu}\mathcal{H}_{\text{nuc.}}\right),$$

$$\hat{\boldsymbol{\mu}} := -\mu_0\hat{\boldsymbol{\sigma}}; \qquad \mathcal{H}_{\text{nuc.}} := \operatorname{rot}\mathbf{A}; \qquad \mathbf{A} := -\left[\hat{\boldsymbol{\mu}}_p \times \boldsymbol{\nabla}\right]\frac{1}{r},$$

где $\hat{\mu}_p = \mu_p \hat{\sigma}_p$ - оператор магнитного момента протона, $\mu_0 = \frac{e\hbar}{2mc}$ - магнетон Бора. Таким образом,

$$\hat{V}^{\text{hyp-f}} = -\mu_0 \mu_p \hat{\sigma} \left[\nabla \times \left[\hat{\sigma}_p \times \nabla\right]\right] \frac{1}{r} = -\mu_0 \mu_p \hat{\sigma} \left[\hat{\sigma}_p \Delta - \left(\hat{\sigma}_p \nabla\right) \nabla\right] \frac{1}{r}.$$

Тут скалярное произведение опущено, потому что нас интересует просто оценка величины.

Применим теорию возмущений. Имеем:

$$\hat{\mathrm{H}}^{(0)} = \hat{\mathbf{p}}^2/(2m) - e^2/r,$$

$$\psi^{(0)}\left(\mathbf{r}, s, s_p\right) = \psi_{100}(\mathbf{r}) \cdot \chi\left(s, s_p\right), \qquad \psi_{100}(\mathbf{r}) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

Получаем:

$$E^{(1)}_{\text{hyp-f}} = \int d^3x \chi^+ \psi^*_{100}(\mathbf{r}) \hat{V}^{\text{hyp-f}} \psi_{100}(\mathbf{r}) \chi.$$

$\psi_{100}(\mathbf{r})$ сферически симметрично, поэтому для поправки нужно усреднить по направлениям $\hat{V}^{\text{hyp-f}}$, то есть нужно нужно заменить $\nabla_i \nabla_j \to \delta_{ij}\Delta/3$. Получим:

$$E^{(1)}_{\text{hyp-f}} = \frac{8\pi}{3} \mu_0 \mu_p |\psi_{100}(0)|^2 \chi^+ \cdot \hat{\sigma}\hat{\sigma}_\rho \cdot \chi.$$

Здесь мы отняли два слагаемых и воспользовались тем, что $\Delta(1/r) = -4\pi\delta(\mathbf{r})$.

Поскольку $(\hat{\sigma}\hat{\sigma}_\rho) = 2\hat{S}^2 - 3\cdot\hat{1}$ (???? откуда это???), то правильными функциями нулевого приближения будут собственные функции оператора квадрата суммарного спина $\hat{\mathbf{S}} = \left(\hat{\sigma} + \hat{\sigma}_p\right)/2$ (т. е. ψ_{SM}, см. задачу 2.10.1 (?? там мб пояснения??)). С учетом того, что $|\psi_{100}(0)|^2 = \left(\pi a^3\right)^{-1}$, получим

$$E^{(1)}_{\text{hyp-f}} = \frac{8}{3} \mu_0 \mu_p \frac{1}{a^3} (2S(S+1) - 3) = \begin{cases} \frac{8}{3}\frac{\mu_0\mu_p}{a^3}, & S = 1, \\ -8\frac{\mu_0\mu_p}{a^3}, & S = 0. \end{cases}$$

Таким образом, исходный уровень энергии расщепляется на два в соответствии со значением суммарного спина электрона и протона, причем один из этих уровней трехкратно вырожден по проекции суммарного спина ($S = 1, M = 0, \pm 1$), а второй уровень - невырожденный ($S = 0$).

Численно $\Delta\nu_{\text{теор}} = \frac{E_{S=1} - E_{S=0}}{h} = 1417$МГц. Данное теоретическое значение отличается от экспериментально измеренного $\Delta\nu_{\text{эксп}} = 1420$ МГц. Причина расхождения результатов состоит в том, что в действительности магнитный момент электрона не равен в точности магнетону Бора μ_0, а отличается от него на величину $\Delta\mu\mu_0$, называемую аномальным магнитным моментом.

Б-2.11.5 Водород в магнитном поле с учетом сверхтонкого расщепления (??!!)

Найти уровни энергии атома водорода в основном (1s) состоянии в однородном магнитном поле. Учесть сверхтонкую структуру.

Solution

Суть решения в том, что

(!!! нужно разобраться с эффектами Зеемана !!!??)

В задаче рассматривается эффект Зеемана для основного состояния атома водорода с учетом его сверхтонкой структуры.

Пусть атом водорода в основном состоянии помещен в магнитное поле $\mathcal{H} = \{0, 0, \mathcal{H}\}$. После проведения стандартных преобразований гамильтониан принимает вид

$$\hat{\mathrm{H}} = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{e^2}{r} + \hat{\mathrm{V}}^{\text{свл.}} + h\Omega\left(\hat{I}_z + 2\hat{\mathrm{S}}_z\right).$$

где $\hat{\mathrm{V}}^{\text{свл.}}$ - поправка сверхтонкого взаимодействия,

$$\hat{V}^{\text{hyp-f}} = -\mu_0 \mu_p \hat{\sigma} \left[\nabla \times \left[\hat{\sigma}_p \times \nabla\right]\right] \frac{1}{r} = -\mu_0 \mu_p \hat{\sigma} \left[\hat{\sigma}_p \Delta - \left(\hat{\sigma}_p \nabla\right) \nabla\right] \frac{1}{r}.$$

также $\Omega = e\mathcal{H}/(2mc)$ - ларморова частота, $\hat{I}_z$ и $\hat{\mathrm{s}}_z$ - операторы проекции орбитального момента и спина электрона на ось z. Мы пренебрегли в (1) квадратичным по полю $\mathcal{H}$ членом, считая его вклад в поправку к энергии малым по сравнению с линейным. Это можно сделать при $\mathcal{H} \ll 10^9$ Гс.

В качестве оператора возмущения выберем $\hat{\mathrm{V}}_{\mathscr{H}} = \hbar\Omega\left(\hat{I}_z + 2\hat{\mathrm{s}}_z\right)$. Гамильтониан невозмущенной задачи $\hat{\mathrm{H}}^{(0)}$ включает сверхтонкое взаимодействие $\hat{\mathrm{V}}^{\text{свл.}}$, поэтому в нулевом приближении мы имеем два уровня с энергиями $E_0 + \Delta E_{0,1}$. Здесь $E_0 = -e^2/(2a)$ - энергия основного состояния атома водорода, $\Delta E_{0,1}$ - поправки сверхтонкой структуры

$$E^{(1)}_{\text{hyp-f}} = \frac{8}{3}\mu_0\mu_p\frac{1}{a^3}(2S(S+1)-3) = \begin{cases} \frac{8}{3}\frac{\mu_0\mu_p}{a^3}, & S=1, \\ -8\frac{\mu_0\mu_p}{a^3}, & S=0. \end{cases}$$

Волновые функции невозмущенной задачи имеют вид $\psi^{(0)} = \psi_{100}(\mathbf{r})\psi_{SM}$, где $\psi_{100}(\mathbf{r})$ - координатная волновая функция основного состояния атома водорода, ψ_{SM} - спиновые функции электрона и протона (задачи 2.10.1 и 2.11.4 (!??!?)).

Поскольку $\langle\psi_{100}|\hat{I}_z|\psi_{100}\rangle = 0$, то вся содержательная часть будет касаться вычислений со спиновыми функциями. Обозначим состояния следующим образом: $|1\rangle = |\psi_{00}\rangle, |2\rangle = |\psi_{10}\rangle, |3\rangle = |\psi_{11}\rangle, |4\rangle = |\psi_{1-1}\rangle$. Заметим, что последние три состояния относятся к трехкратно вырожденному уровню с $S = 1$, а состояние $|1\rangle$ - к невырожденному уровню с $S = 0$. Отличные от нуля матричные элементы оператора возмущения равны

$$\langle 1|\hat{\mathrm{V}}_{\mathscr{H}}|2\rangle = \langle 2|\hat{\mathrm{V}}_{\mathscr{H}}|1\rangle = \langle 3|\hat{\mathrm{V}}_{\mathscr{H}}|3\rangle = -\langle 4|\hat{\mathrm{V}}_{\mathscr{H}}|4\rangle = \hbar\Omega.$$

Учитывая малость сверхтонкого расщепления, мы можем считать невозмущенные уровни энергии близкими. Поэтому, записывая секулярное уравнение, включим в него наряду с матричными элементами (2) также и сверхтонкие поправки $\Delta E_{0,1}$:

$$\begin{vmatrix} \Delta E_0 - E^{(1)} & \hbar\Omega & 0 & 0 \\ \hbar\Omega & \Delta E_1 - E^{(1)} & 0 & 0 \\ 0 & 0 & \Delta E_1 + \hbar\Omega - E^{(1)} & 0 \\ 0 & 0 & 0 & \Delta E_1 - \hbar\Omega - E^{(1)} \end{vmatrix} = 0$$

Отсюда получаем (?? пока верю этому.)

$$E^{(1)}_{1,2} = \frac{1}{2}\left\{(\Delta E_0 + \Delta E_1) \mp \sqrt{(\Delta E_1 - \Delta E_0)^2 + 4(\hbar\Omega)^2}\right\}.$$
$$E^{(1)}_{3,4} = \Delta E_1 \pm \hbar\Omega.$$

Проведем анализ результатов. Во-первых, состояния $|3\rangle = |\psi_{11}\rangle$ и $|4\rangle = |\psi_{1-1}\rangle$, относящиеся к уровню сверхтонкой структуры с $S = 1$, получают линейные по полю поправки $\pm\hbar\Omega$. Тем самым снимается вырождение по проекции суммарного спина M, уровень энергии с $S = 1$ расщепляется на три уровня.

В слабом поле, когда вклад магнитного поля много меньше вклада сверхтонкого взаимодействия ($\hbar\Omega \ll \Delta E_{\text{са}\tau} = \Delta E_1 - \Delta E_0$, это справедливо для $\mathcal{H} \ll 10^3$ Гс), поправки получают также состояния $|1\rangle = |\psi 00\rangle$ и $|2\rangle = |\psi_{10}\rangle$. Эти состояния относятся к разным уровням сверхтонкой структуры: $S = 0$ и $S = 1$, но они отвечают одному и тому же значению проекции суммарного спина $M = 0$ (рис. 2.12). Данные поправки квадратичны по полю:

$$E^{(1)}_{1,2} \simeq \Delta E_{0.1} \mp \frac{(\hbar\Omega)^2}{\Delta E_1 - \Delta E_0},$$

но ввиду наличия малого знаменателя $\Delta E_1 - \Delta E_0$ (малости сверхтонкого расщепления) вклад этих поправок может быть существенно больше, чем вклад отброшенного квадратичного по $\mathcal{H}$ члена в гамильтониане.

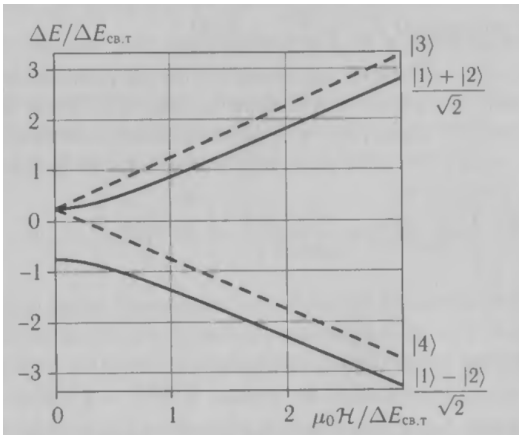


Рис. 2.12. Эффект Зеемана с учетом сверхтонкой структуры для основного состояния атома водорода ($\mu_0\mathscr{H} = \hbar\Omega, \Delta E_{\text{hyp-f}} = \Delta E_1 - \Delta E_0$)

В сильном поле, когда $\hbar\Omega \gg \Delta E_1 - \Delta E_0$, поправки, относящиеся к состояниям $|1\rangle$ и $|2\rangle$, равны

$$E^{(1)}_{1,2} \simeq \mp\hbar\Omega,$$

а правильные функции

$$\tilde{\psi}_{1,2} = \frac{1}{\sqrt{2}}\left(\psi_{00} \mp \psi_{10}\right)$$

описывают состояния, которые характеризуются значениями проекций электронного и протонного спина на направление магнитного поля по отдельности.

Заметим, что в данном приближении состояния $|3\rangle$ и $|4\rangle$ получают поправки

$$E^{(1)}_{3,4} \simeq \pm h\Omega,$$

и при этом в состояниях $|3\rangle = |\psi_{11}\rangle$ и $|4\rangle = |\psi_{1-1}\rangle$ проекции электронного и протонного спина на ось z также имеют определенные значения (как и в состояниях $\widetilde{\psi}_{1,2}$).

Это и понятно, ибо в случае сильного поля можно вначале учесть взаимодействие с полем, а затем, повторно применяя теорию возмущений, - сверхтонкое взаимодействие. Взаимодействие с магнитным полем в (1) влияет только на проекцию спина электрона и не затрагивает спин протона. Поэтому, сопоставляя (4) и (5), мы видим, что в сильном поле (до учета сверхтонкого взаимодействия) мы имеем два двукратно вырожденных (по значениям проекции спина протона) уровня энергии, отвечающие поправкам $E^{(1)}_{1,2} = E^{(1)}_{4,3} \simeq \mp\hbar\Omega$.

Б-2.11.6 Волновые функции с учетом SO-взаимодействия

Для свободного атома водорода написать правильные функции возбужденных состояний с $n = 2$ с учетом спин-орбитального взаимодействия (спин ядра считать равным нулю).

Solution

Суть решения в том, что (???)

Гамильтониан атома водорода с учетом релятивистских и спиновых поправок приведен в решении задачи 2.9.7, см. формулу (11).

Поправки содержат оператор спин-орбитального взаимодействия, который с учетом $U(r) = -Ze^2/r$ может быть записан в виде

$$\hat{\mathrm{V}}^{\mathrm{so}} = \frac{e^2\hbar^2}{2m^2c^2}\frac{(\hat{\mathbf{s}}\hat{\mathbf{i}})}{r^3} = A(r)(\hat{\mathbf{s}}\hat{I}),$$

где $\hat{\mathbf{i}}$ и $\hat{\mathbf{s}}$ - операторы орбитального и спинового моментов электрона. Правильные функции нулевого приближения должны быть собственными функциями операторов, являющихся точными интегралами движения (т. е. коммутирующих не только с $\hat{\mathrm{H}}^{(0)} = \hat{\mathbf{p}}^2/(2m) - e^2/r$, но и с $\hat{\mathrm{V}}^{so}$, играющим роль оператора возмущения). Стандартные решения уравнения Шредингера, пропорциональные сферическим функциям $\psi_{nlm}(\mathbf{r}) = R_{nl}(r)Y^{(m)}_l(\theta,\varphi)$, не подходят для наших целей, ибо эти функции являются собственными для оператора $\hat{I}_z$, а данный оператор, как легко проверить, не коммутирует с $\hat{V}^{\mathrm{co}}$: $\left[(\hat{s}\hat{i}), \hat{I}_z\right] \neq 0$.

Однако оказывается, что $\left[(\hat{\mathbf{s}}\hat{\mathbf{s}}), \hat{\mathrm{j}}_z\right] = 0$, т. е. точным интегралом движения является проекция на ось z полного углового момента $\hat{\mathrm{j}}_z = \hat{I}_z + \hat{\mathrm{s}}_z$. Это значит, что искомые функции должны быть общими собственными функциями для полного набора наблюдаемых $\hat{\mathrm{H}}^{(0)}, \hat{I}^2, \hat{\mathrm{s}}^2, \mathrm{j}^2, \hat{\mathrm{j}}_z$, к которому можно перейти от стандартного набора $\hat{\mathrm{H}}^{(0)}, \hat{I}^2, \hat{\mathrm{s}}^2, \hat{\mathrm{s}}_z, \hat{I}_z$. Эти два набора эквивалентны, ибо по сути данный переход есть не что иное, как задача сложения моментов: $\hat{\mathbf{j}} = \hat{\mathbf{i}} + \hat{\mathbf{s}}$.

Итак, правильный вектор состояния атома водорода должен определяться следующими квантовыми числами: $|nljm_j\rangle$, где мы опустили квантовое число s, потому что оно всегда имеет значение $s = 1/2$. В координатном представлении этим векторам отвечают функции, найденные в решении задачи 2.10.3. Воспользуемся результатами данной задачи и конкретизируем их для $n = 2$.

Для $n = 2$ имеется восемь состояний, из которых в двух состояниях орбитальный момент равен нулю. Поэтому волновые функции этих состояний можно записать в виде

$$\Psi^{\frac{1}{2}}_{2,0,+1/2}(\mathbf{r}) = R_{20}(r)\begin{pmatrix} Y^{(0)}_0 \\ 0 \end{pmatrix}, \quad \Psi^{\frac{1}{2}}_{2,0,-1/2}(\mathbf{r}) = R_{20}(r)\begin{pmatrix} 0 \\ Y^{(0)}_0 \end{pmatrix}.$$

Соответствующие векторы состояний имеют вид

$$|2,0,1/2,\pm 1/2\rangle = |2,0,0\rangle|\pm\rangle,$$

где $|\pm\rangle$ - собственные векторы оператора $\hat{s}_z$, а в представлении, где $\hat{s}_z$ диагонален, им соответствуют функции $\chi_{\pm 1/2}$ (II.26).

Для значения орбитального квантового числа $l = 1$ возможны два состояния с полным моментом $j = 1/2$ и четыре состояния с $j = 3/2$. Используя общие результаты задачи 2.10.3, получаем

$$\Psi^{\frac{1}{2}}_{2,1,+1/2}(\mathbf{r}) = R_{21}(r)\begin{pmatrix} -\frac{1}{\sqrt{3}}Y_1^{(0)} \\ \sqrt{\frac{2}{3}}Y_1^{(1)} \end{pmatrix}, \quad \Psi^{\frac{1}{2}}_{2,1,-1/2}(\mathbf{r}) = R_{21}(r)\begin{pmatrix} -\sqrt{\frac{2}{3}}Y_1^{(-1)} \\ \frac{1}{\sqrt{3}}Y_1^{(0)} \end{pmatrix},$$

или в виде векторов состояний:

$$|2,1,\frac{1}{2},+\frac{1}{2}\rangle = \frac{1}{\sqrt{3}}\Big[\sqrt{2}|2,1,+1\rangle|-\rangle - |2,1,0\rangle|+\rangle\Big].$$

$$|2,1,\frac{1}{2},-\frac{1}{2}\rangle = \frac{1}{\sqrt{3}}\Big[|2,1,0\rangle|-\rangle - \sqrt{2}|2,1,-1\rangle|+\rangle\Big].$$

Соответственно для полного момента $j = 3/2$ мы должны записать четыре состояния. Выпишем только два состояния с положительными проекциями полного момента (остальные два легко написать самостоятельно):

$$\Psi^{(3/2)}_{2,1,+3/2}(\mathbf{r}) = R_{21}(r)\begin{pmatrix} Y_1^{(1)} \\ 0 \end{pmatrix}, \quad \Psi^{(3/2)}_{2,1,+1/2}(\mathbf{r}) = R_{21}(r)\begin{pmatrix} \sqrt{\frac{2}{3}}Y_1^{(0)} \\ \frac{1}{\sqrt{3}}Y_1^{(1)} \end{pmatrix},$$

или в виде векторов состояний:

$$|2,1,3/2,+3/2\rangle = |2,1,+1\rangle|+\rangle$$
$$|2,1,3/2,+1/2\rangle = \frac{1}{\sqrt{3}}(\sqrt{2}|2,1,0\rangle|+\rangle + |2,1,+1\rangle|-\rangle).$$

Б-2.11.7 Тонкое расщепление водорода (!!!)

Найти величину тонкого расщепления состояния атома водорода с главным квантовым числом n и орбитальным квантовым числом l. Выразить величину этого расщепления в атомных единицах энергии. Нарисовать схему расщепленных уровней с $n = 3$.

Solution

Эта задача по теории: берем гамильтониан Дирака для кулоновского поля в нерелятивистском приближении, раскладываем по теории возмущений. Для именно этой задаче и обсуждали мы релятивистскую квантовую механику.

(напишу тут пару ключевых формул)

Получаем в итоге формулу Зоммерфельда для уровней энергии атома водорода с учетом релятивистских поправок:

$$E_{nj} = -\frac{Z^2}{2n^2}\left(\frac{e^2}{a}\right)\left\{1 + \frac{Z^2\alpha^2}{n^2}\left[\frac{n}{j+1/2} - \frac{3}{4}\right]\right\}.$$

где $n = 1, 2, \ldots$ - главное квантовое число, $j = l \pm 1/2$ - внутреннее квантовое число.

(дальше выпишу из теории коротко решение)

(?? это пока не понимаю.) В качестве правильных функций невозмущенной задачи выбрать функции, собственные для следующего набора коммутирующих операторов: $\hat{I}^2, \hat{\mathbf{s}}^2, \hat{\mathrm{j}}^2, \hat{\mathrm{j}}_z$, где $\hat{\mathbf{j}} = \hat{\mathbf{i}} + \hat{\mathbf{s}}$ - полный угловой момент электрона, см. задачу 2.10.3.

18.1.4 Problems about Special Effects in Atoms 2

Б-2.11.11 Основное состояние водорода вариацией

Вычислить энергию основного состояния атома водорода из вариационного принципа. В качестве пробных функций взять:

а) $\psi(r) = \left(\pi a^3\right)^{-1/2}\exp(-r/a)$

б) $\psi(r) = \left(\pi b^2\right)^{-3/4}\exp\left(-r^2/2b^2\right)$.

Определить параметры a и b.

Solution

Суть решения в том, что (?? применяем вар метод и все???)
Параметры функции $\psi(\mathbf{r})$, выбранной для применения вариационного метода, определяются, исходя из того, чтобы вычисленное при помощи этой функции среднее значение гамильтониана

$$\langle\hat{\mathrm{H}}\rangle = \int \psi^*(\mathbf{r})\hat{\mathrm{H}}\psi(\mathbf{r})d^3x, \text{ где } \hat{\mathrm{H}} = -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{r},$$

имело бы минимум при условии, что функция $\psi(\mathbf{r})$ является нормированной. Вычисляя интегралы и находя минимумы для средних значений гамильтониана $\langle\hat{\mathrm{H}}\rangle$, получаем:
(!?!?!? ну вот нужно сесть и сделать это!!!)
случай а) $a = \frac{\hbar^2}{me^2}$, $\quad \langle\hat{\mathrm{H}}\rangle = -\frac{1}{2}\frac{me^4}{\hbar^2}$ (точное решение);
случай б) $b = \frac{3\sqrt{\pi}}{4}\frac{\hbar^2}{me^2}$, $\quad \langle\hat{\mathrm{H}}\rangle = -\frac{4}{3\pi}\frac{me^4}{\hbar^2} \simeq -\frac{1}{2{,}36}\frac{me^4}{\hbar^2}$.

Б-2.11.12 Диамагнитная восприимчивость гелия вариацией

Найти диамагнитную восприимчивость атома гелия в основном состоянии, исходя из волновой функции вида
а) $\psi(r) = \left(\pi a^3\right)^{-1/2}\exp(-\frac{r}{a})$;
б) $\psi(r) = \left(\pi b^2\right)^{-3/4}\exp\left(-\frac{r^2}{2b^2}\right)$.
Определить параметры a и b.

Solution

Суть решения в том, что
2.11.12. Гамильтониан атома гелия, записанный в атомной системе единиц, имеет вид

$$\hat{\mathrm{H}} = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}},$$

где $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. В выражении (1) первые два слагаемых описывают кинетическую энергию электронов, третье и четвертое слагаемые притяжение электронов к ядру (для гелия $Z = 2$) и последнее слагаемое описывает кулоновское отталкивание электронов. Первая часть задачи предполагает минимизацию среднего значения гамильтониана (1), найденного при помощи пробной функции $\psi \sim \exp\left[-Z'\left(r_1 + r_2\right)\right]$, и нахождение значения вариационного параметра Z'. Нормируем пробную функцию и получаем

$$\psi = \frac{Z'^3}{\pi}e^{-Z'(r_1+r_2)}.$$

При вычислении среднего значения гамильтониана $\langle\hat{\mathrm{H}}\rangle$ нам встретятся интегралы

$$\langle\frac{1}{r_1}\rangle = \langle\frac{1}{r_2}\rangle = Z',$$

по поводу их вычисления - см. задачу 2.6.4, а также интеграл

$$\langle\frac{1}{r_{12}}\rangle = \left(\frac{Z'^3}{\pi}\right)^2\int dr_1 dr_2\frac{r_1^2 r_2^2 d\Omega_1 d\Omega_2 e^{-2Z'(r_1+r_2)}}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2\cos\theta}}.$$

В интеграле (3) зафиксируем вначале значение $\mathbf{r}_1$ и проинтегрируем по угловым переменным, относящимся к r_2, совместив ось z с направлением вектора $\mathbf{r}_1$. В результате получим

$$2\pi\int\limits_0^\pi \frac{\sin\theta d\theta}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2\cos\theta}} = \begin{cases}\frac{4\pi}{r_1}, & r_1 > r_2,\\ \frac{4\pi}{r_2}, & r_2 > r_1.\end{cases}$$

С учетом данного результата приводим интеграл (3) к виду

$$\langle\frac{1}{r_{12}}\rangle = \left(4Z'^3\right)^2\left\{\int\limits_0^\infty r_1 e^{-2Z'r_1}dr_1\int\limits_0^{r_1} r_2^2 e^{-2Z'r_2}dr_2 + \int\limits_0^\infty r_2 e^{-2Z'r_2}dr_2\int\limits_0^{r_2} r_1^2 e^{-2Z'r_1}dr_1\right\} =$$
$$= Z'\left(2 - \frac{11}{8}\right) = \frac{5}{8}Z'.$$

Собирая далее результаты (2) и (4), получаем для среднего значения $\langle\hat{\mathrm{H}}\rangle$ следующее выражение:

$$\langle\hat{\mathrm{H}}\rangle = -2ZZ' + \frac{5}{8}Z' + Z'^2,$$

где мы учли, что $-\langle\Delta_1\rangle = -\langle\Delta_2\rangle = Z'^2$, как это следует из решения задачи 2.6.4. Заметим, что наша пробная функция фактически есть произведение двух функций основного состояния атома водорода с единственным отличием $Z \to Z'$, поэтому использование результатов задачи 2.6.4 является корректным. Минимизируем $\langle\hat{\mathrm{H}}\rangle$ и находим

$$Z' = Z - \frac{5}{16},$$

т. е. для гелия $Z' = 27/16$. Полученное значение Z' имеет прозрачный физический смысл - это значение эффективного заряда ядра, которое «чувствует» электрон при движении в общем кулоновском поле ядра и второго электрона - часть заряда ядра Z экранируется вторым электроном.

Найдем далее диамагнитную восприимчивость основного состояния гелия. Запишем общий вид гамильтониана для атома гелия в однородном внешнем магнитном поле (в обычной системе единиц):

$$\hat{\mathrm{H}} = \hat{\mathrm{H}}_0 + \frac{e\hbar}{2mc}\mathcal{H}(\hat{\mathbf{L}} + 2\hat{\mathbf{S}}) + \frac{e^2}{8mc^2}\sum_{a=1,2}\left[\mathcal{H}\times\mathbf{r}_a\right]^2,$$

обозначения совпадают с обозначениями задачи 2.11.10. Заметим, что в основном состоянии гелия $L = S = 0$, поэтому линейное по $\mathcal{H}$ слагаемое не дает вклада в поправку к энергии. Следовательно,

$$E^{(1)} = \frac{e^2}{8mc^2}\langle\sum_{a=1,2}[\mathcal{H}\times\mathbf{r}_a]^2\rangle = \frac{e^2}{8mc^2}\frac{2}{3}\mathcal{H}^2\sum_{a=1,2}\langle r_a^2\rangle,$$

где угловые скобки $\langle ...\rangle$ означают усреднение по состоянию с пробной функцией с зарядом Z'. Диамагнитная восприимчивость равна

$$\chi = -\frac{\partial^2 E^{(1)}}{\partial\mathcal{H}^2} = -\frac{e^2}{6mc^2}\sum_{a=1,2}\langle r_a^2\rangle = -\frac{e^2}{6mc^2}\frac{a^2}{Z'^2} = -\frac{1}{Z'^2}a^3\alpha^2,$$

где $\alpha = e^2/(\hbar c) \simeq 1/137$ - постоянная тонкой структуры. Численное значение восприимчивости: $\chi = -2,77\cdot 10^{-30}$ см^3.

Б-2.11.13 Парамагнетизм Ван Флека (?)

Показать, что газ атомов, обладающих в основном состоянии полным моментом $J = 0$, но при этом $L = S \neq 0$, парамагнитен (парамагнетизм Ван Флека).

Solution

Суть решения в том, что

В этом случае поправка первого порядка для зеемановского взаимодействия $\hat{V}_Z$ (см. (II.61)) равна нулю. Оценим поправку второго порядка для возмущения $\hat{V}_Z$ к уровню энергии атома с $L = S \neq 0$ и $J = 0$. Поправка второго порядка содержит энергетический знаменатель, равный разности энергии основного терма и соответствующего возбужденного состояния. Среди всех возможных энергетических знаменателей следует учесть только те, которые относятся к одной конфигурации основного терма, поскольку расстояние между уровнями энергии с одной и той же конфигурацией имеет величину порядка $\alpha^2 E_0 \sim A$, где A - эффективная величина спин-орбитального взаимодействия. Таким образом, оценка поправки второго порядка есть

$$\Delta E^{(2)} \approx \sum_{J,M_J}\frac{|\langle L,S,J,M_J|\hat{V}_Z|L,S,0,0\rangle|^2}{E_{LSO} - E_{LSJ}} \sim \frac{\mu_0^2\mathcal{H}^2}{A}.$$

Легко видеть, что $|\Delta E_{\mathrm{Z}}^{(2)}|/|\Delta E_{\mathrm{D}}^{(1)}| > 1$, где $E_{\mathrm{D}}^{(1)}$ - поправка первого приближения для диамагнитного взаимодействия (II.62). Вспомним также, что поправка второго приближения к основному состоянию всегда отрицательна, поэтому газ таких атомов, находящихся в основном состоянии с $J = 0$ и $L = S \neq 0$, будет парамагнитным.

Б-2.11.14 Свойства молекулы водорода (??????)

Определить зависимость вращательного квантового числа молекулы водорода H_2 от суммарного спина S протонов.

Solution

Суть решения в том, что

Б-2.11.15 Спектр двухатомной молекулы, описываемой потенциалом Кратцера (?)

Найти энергетический спектр двухатомной молекулы, считая, что энергия взаимодействия ядер описывается модельным потенциалом Кратцера:

$$U(r) = -2D\left(\frac{b}{r} - \frac{b^2}{2r^2}\right)$$

Solution

Суть решения в том, что

Б-2.11.16 $p\mu$-атом

Отрицательный мюон захватывается протоном, образуя $p\mu$-атом, «боровский радиус» которого в 207 раз меньше соответствующего радиуса атома водорода. На таких расстояниях уже оказываются существенными ядерные силы, и мюон может захватиться протоном. Однако скорость захвата существенно зависит от величины суммарного спина μ-атома $\mathbf{S} = \mathbf{s}_\mu + \mathbf{s}_p$. Таким образом, время жизни отрицательного мюона в среде сильно зависит от величины суммарного спина S. Образовавшийся медленный $p\mu$-атом, как и нейтрон, взаимодействует с ядрами среды контактным образом, однако при этом взаимодействии следует учитывать также магнитное сверхтонкое взаимодействие, которое, как и для атома водорода в s-состоянии имеет изотропный контактный характер. Построить контактный оператор сверхтонкого взаимодействия $p\mu$-атома с ядром, обладающим спином I, при котором изменяется суммарный спин S $p\mu$-атома.
(вроде кривовато задача сформулирована, перепишу потом ее.)

Solution

Суть решения в том, что

18.1.5 Basic Problems about Hydrogen Atoms 1

Мартинсов,Смирнов-5.2. Водорода с массой ядра

Покажите, как изменятся частота излучения атома водорода с учетом конечной величины массы ядра. $m_0 r_e = M r_\mathrm{r}$, аде $m_0 u M$, соответственно, массы электрона и ядра.

Solution

(???)
Из равенства ускорений электрона и ядра вытекает условие равенства их угловых скоростей вращения

$$\frac{\mathrm{v}_e}{r_e} = \frac{\mathrm{v}_\mathrm{B}}{r_\mathrm{a}} = \omega.$$

${}^{2\partial}\mathbf{v}_e{}^{u}\mathbf{v}_\mathrm{g}$ - скорости электрона и ядра, соответственно. С учетом движения ядра, момент импульса атома

$$L = m_0 \mathrm{v}_e r_e + M \mathrm{v}_\pi r_\mathrm{a} = m_0 \omega r_e^2 + M \omega r_\mathrm{a}^2$$

$$\begin{cases} m_0\omega^2 r_e = \frac{e^2}{4\pi\varepsilon_0 (r_e + r_\pi)^2}, \\ m_0 \omega \alpha_e^2 + M\omega r_\pi^2 = n\hbar, \quad n = 1, 2, 3, ... \end{cases}$$

Если расстояние между электроном и ядром обозначить через $r = r_e + r_\mathrm{g} = r_e\,(1 + m_0/M)$, то после преобразований эти соотношения запишутся в виде

$$\begin{cases} \mu\omega^2 r = \frac{e^2}{4\pi\varepsilon_0 r^2}, \\ \mu\omega^2 = n\hbar, \quad n = 1, 2, 3, ... \end{cases}$$

здесь введена приведенная масса системы "электрон-ядро"

$$\mu = \frac{m_0 M}{m_0 + M}$$

$$\mu = \frac{m_0 M}{m_0 + M}$$

Решая полученную систему уравнений, находим для стационарных состояний атома $(n = 1, 2, ...)$

$$r_n = \frac{4\pi\varepsilon_0\hbar^2 n^2}{\mu e^2} \quad \text{и} \quad \omega_n = \frac{\mu e^4}{16\pi^2\varepsilon_0^2\hbar^3 n^3}.$$

Полная энергия атома

$$E = \frac{m_0 \mathrm{v}_e^2}{2} + \frac{M \mathrm{v}_\mathrm{g}^2}{2} - \frac{e^2}{4\pi\varepsilon_0 (r_e + r_\mathrm{a})} = \frac{\mu\omega^2 r}{2} - \frac{e^2}{4\pi\varepsilon_0 r}.$$

Подставляя сюда значения ${r_n}^u\boldsymbol{\omega}_n$, получаем формулу квантования энераии атома

$$E_n = -\frac{\mu e^4}{32\pi^2\varepsilon_0^2\hbar^2} \cdot \frac{1}{n^2}, n = 1, 2, ...$$

Отсюда находим частоты спектральных линий излучения такого атома:

$$\omega_{nk} = \frac{E_k - E_n}{\hbar} = R_\mathrm{M}\left(\frac{1}{n^2} - \frac{1}{k^2}\right)$$

где модифицированная постоянная Ридберга

$$R_\mathrm{M} = \frac{\mu e^4}{32\pi^2\varepsilon_0^2\hbar^3} = \frac{R}{1 + \frac{m_0}{M}}$$

был открыт изотоп тяжелого водорода - дейтерий D, для которого $M_D = 2M_H$

Spaldin-3.1(20 sec) Moment along the field axis

Calculate the allowed values of the magnetic moment along the field axis of an atom which has $J = 1$ and $g = 2$.

Solution

The total magnetic moment of an atom is $m = g\sqrt{J(J+1)}\mu_\mathrm{B}$, and $m_z = -gM_J\mu_\mathrm{B}$.
We have $J = 1$, $\sqrt{J(J+1)} = \sqrt{2}$, $M_J = -1, 0,$ or 1, $g = 2$. So

$$|m| = 2\sqrt{2}\mu_\mathrm{B}, \qquad m_z = -2\mu_\mathrm{B}, \quad 0, \text{ or } +2\mu_\mathrm{B}.$$

Note that in all cases the component along the field direction is less than the total magnetic moment.
(кст, еще 1ю часть доработаю для этой задачи!!!!)

O3.1-4.1

Частица находится в центральном поле силового центра с потенциальной энергией $U = -C/r^s$, где C - положительная постоянная, а r - расстояние от силового центра. Исходя из соотношения неопределённостей, показать, что при $s > 2$ возможны стационарные состояния частицы со сколь угодно большими по абсолютной величине отрицательными собственными значениями полной энергии. Частица при этом условии будет переходить на нижележащие энергетические уровни - произойдет ее «падение» в точку $r = 0$, т.е. на силовой центр. Если же $s < 2$, то наиболее низкий энергетический уровень будет иметь конечное значение полной энергии, Пользуясь этими результатами, объяснить возможность существования атомов, например атома волорода.

4.

1* Решение. Пусть частица локализована вблизи силового центра внутри сферы, радиус которой r. Ее потенциальная энергия будет порядка $-C/r^s$. Неопределенность координаты будет порядка r, а, следовательно, неопределенность импульса - порядка $\hbar/r$. Такого же порядка будет и сам импульс. Следовательно, средняя кинетическая энергия будет порядка $\hbar^2/mr^2$, а полная энергия

$$\mathscr{E} \sim \frac{\hbar^2}{mr^2} - \frac{C}{r^s}.$$

Если $s > 2$, то $\mathfrak{G}$ может принимать сколь угодно большие отрицательные значения. Но в таком случае должны существовать и уровни энергии со

сколь угодно большими по абсолютной величине отрицательными значениями $\mathscr{E}$ - произойдет падение частицы на силовой центр. Если же $s < 2$, то сколь угодно большие по абсолютной величине значения $\mathscr{E}$ невозможны, поэтому невозможно падение на силовой центр и возможно образование связанного состояния с $\mathscr{E} < 0$.

О3.1-4.2

Показать, что в пределе, когда главные числа в атоме водорода стремится к бесконечности, движение электрона переходит в классическое движение по круговой орбите-

(???)

О3.1-4.3 Третий закон Кеплера из квантовой механики (???)

Классические формулы следуют из квантовых в пределе как и в задаче Кеплера, потенццальная энергия $U(r) \propto \frac{1}{r}$. из квантовых формул для уровней энергии $\wp_n = -\mathrm{Ry}/n^2$ и радиусов состояний $r_n = an^2$ электрона в атоме водорода, получить для больших n третий закон Кеплера.

(??? тут кривое скорее всего условие)

4.

3. $\frac{r^3}{T^2} = \frac{e^2}{4\pi^2 m} = \text{const}$. (Классический закон Кеплера в системе Солн-це-Земля $\frac{r^3}{T^2} = \frac{\gamma M_\text{C}}{4\pi^2} = \text{const}$.

О3.1-4.4 Простейшие свойства решения атома водорода (20 секунд)

Показать, что среди сферически симметричных решений уравнения Шредингера для водородоподобного атома, конечных при $r = 0$ и обращающихся в нуль при $r = \infty$, имеется экспоненциальное решение $e^{-\alpha r}$. Найти постоянную α и энергию атома в рассматриваемом состоянии. Что это за состояние?

4.

4. $\psi \propto e^{-\alpha r}$, где $\alpha = \frac{mZe^2}{\hbar^2} = \frac{1}{r_1}, r_1$ - радиус первой боровской орбиты водородоподобного атома, а функция ψ - с точностью до нормировочной константы - описывает основное состояние водородоподобного атома $\left(\psi_1 = \frac{1}{\sqrt{\pi r_1^3}} e^{-r/r_1}\right)$. $\mathscr{E}_1 = -\frac{mz^2e^4}{2\hbar^2}$.

О3.1-4.5

Найти объемную плотность вероятности нахождения электрона в водородоподобном атоме для основного состояния.

4.

5. $|\psi|^2 = \frac{q^2}{4\pi} e^{-qr}$, где $q = \frac{2mZe^2}{\hbar^2}$.

О3.1-4.6(30 sec) Плотность вероятности в атоме водорода

Найти радиальную плотность вероятности нахождения электрона в водородоподобном атоме для основного состояния. При каких значениях r эта величина достигает максимума.

4.

6. $4\pi r^2|\psi|^2 = q^3 r^2 e^{-qr}$, где $q = \frac{2mZe^2}{\hbar^2}$. Эта величина максимальна при $r = \frac{2}{q} = \frac{\hbar^2}{mZe^2} = r_1$, где r_1 - радиус первой боровской орбиты.

(1 строчка тут будет вычисления этого интеграла.)

О3.1-4.7(20 sec) среднее расстояние от ядра в $1s$-состоянии

Найти среднее расстояние $\langle r\rangle$ электрона от ядра в $1s$-состоянии водородоподобного атома.

4.

7. $\langle r\rangle = \frac{3}{2} r_1$.

О3.1-4.8(20 sec) среднее обратное расстояние от ядра в $1s$-состоянии

Найти среднее значение обратного расстояния $\langle 1/r\rangle$ электрона от ядра в основном состоянии водородоподобного атома.
(??? формула Крамерса сразу же говорит ответ??? заготовлю их!!!)

О3.1-4.9(30 sec) $\langle U\rangle$ и $\langle T\rangle$ основного состояния водорода

Найти средние значения потенциальной $\langle U\rangle$ и кинетической $\langle T\rangle$ энергий основного состояния водородоподобного атома.
(чет тут теряюсь, прописать лучше нужно темы эти!!! точно первая часть требует доработку по этому, с ходу формулы не готовы! плохо, а что поделать?)

О3.1-4.10(50 sec) Энергия и константы в водороде по затравочной функции

Волновая функция одного из состояний атома водорода имеет вид $\psi = A(1+\alpha r)e^{-\beta r}$, где A, α, β - некоторые константы. Определить величину констант α и β, энергию этого состояния и его квантовые числа.

О3.1-4.11

Определить разрешающую способность R спектрального прибора, необходимую для наблюдения изотопического сдвига спектральных линий дейтерия относительно линий водорода. Какова должна быть ширина b основания призмы из тяжелого флинта с дисперсией $dn/d\lambda = 1000\text{см}^{-1}$ (в диапазоне красного света) в призменном спектрографе, применяемом для обнаружения изотопического сдвига головной линии серии Бальмера?

О3.1-4.12

Серия Лаймана наблюдается в смеси атомарных водорода и трития (ядро атома трития состоит из протона и двух нейтронов). Определить разрешающую способность спектрального прибора, которая достаточна для разрешения изотопической структуры спектральных линий этой серии. Как меняется требуемая разрешающая способность при переходе к другим сериям (Бальмера, Пашена) той же смеси? Можно ли разрешить изотопическую структуру спектральных линий той же смеси в видимой области спектра с помощью стеклянной призмы с основанием $b = 1$ см и дисперсией показателя преломления $dn/d\lambda = 1000\text{см}^{-1}$? Каково должно быть эффективное разрешить и исследовать ту же структуру с помощью интерферометра Фабри-Перо?

О3.1-4.13

Серия Бальмера наблюдается в смеси атомарных водорода и дейтерия. Определить разрешающую способность и число штрихов N дифракционной решетки, которые необходимы для разрешения во втором порядке изотопической структуры спектральных линий этой серии. Как меняется эта разрешающая способность с увеличением номера линии (т. е. с уменьшением длины волны) указанной серии?

О3.1-4.14

В спектрах некоторых звезд наблюдается $m \approx 30$ линий водородной серии Бальмера. При каком наименьшем числе N штрихов дифракционной решетки можно разрешить эти линии в спектре первого порядка?

О3.1-4.15

Кварцевая пластинка, расположенная между скрещенными поляроидами, образует поляризационный фильтр. Разрешенные направления пластинки составляют угол 45° с главными направлениями поляроидов. Какую минимальную толщину должна иметь пластинка, для того чтобы с помощью такого фильтра можно было от делить наиболее длинноволновую линию серии Бальмера для водорода ($\lambda = 656$ нм) от той же линии дейтерия? Показатели преломления для обыкновенного и необыкновенного лучей в кварце $n_0 = 1,5442, n_\text{e} = 1,5533$. Источником света является газоразрядная водородно-дейтериевая лампа.

О3.1-4.16

Каково должно быть минимальное расстояние между зеркалами в интерферометре Фабри-Перо, чтобы по оптическому спектру установить наличие двух изотопов калия $^{39}_{19}$ К и $^{40}_{19}$ К? Коэффициент отражения зеркал по энергии 0,9, энергия ионизации атома калия $W = 4,3$ эВ.

О3.1-4.17

Отрицательные мюоны могут захватываться атомом и замещать в нем электроны электронной оболочки. Практически может замещаться лищь один электрон. Получающиеся в результате такой замены системы называются мезоатомами. Масса мюона $m_\mu = 207m_\text{e}$. Вычислить по теории Бора радиус первой круговой орбиты (К-орбиты) мюона в мезоатоме. Рассчитать энергетические уровни мезоатома. Какое излучение будет наблюдаться при переходе на К-орбиту мюона с более высоких орбит? Почему исследование такого излучения лрименяется для выявления структуры тяжелых атомных ядер? Массой мюона по сравнению с массой ядра пренебречь.

О3.1-4.18

Позитроний представляет собой связанную систему из электрона и его античастицы - позитрона. Найти уровни энергии, энергию ионизации и соответствующую ей длину волны резонансной линии позитрония. Резонансным называют переход из первого возбужденного состояния в основное.

О3.1-4.19 Энергия ионизации по спектру (????)

Длина волны линии H_α водородной серии Бальмера равна $\lambda = 0,656$ мкм. Определить по этим данным энергии ионизации $\mathscr{E}_\text{и}$ позитрония и мюония, находящихся в основном состоянии. Масса мюона $m_\mu = 207m_\text{e}$ (m_e - масса электрона).

4.

19. $\mathscr{E} = 6,8$ эВ (для позитрония) ; $\mathscr{E}_\text{и} = 2,6$ кэВ (для мюония).

О3.1-4.20

Рассчитать энергию излучения $\Delta\mathscr{E}$, испускаемого в мезоатоме водорода (мюония) при переходе мюона с N- на M-оболочку. Как велик радиус 1-й боровской орбиты в этом случае?

4.

20. $\Delta\mathscr{E} = \frac{\mu e^4}{2\hbar^2}\left(\frac{1}{3^2} - \frac{1}{4^2}\right) \approx 125$ эВ, где $\mu = \frac{m_\mu m_\text{p}}{m_\mu + m_\text{p}}$ - приведенная масса мезоатома; $r_\mu = \frac{m_e}{m_\mu} r_1 = 2,8 \cdot 10^{-11}$ cm, где $r_\text{I} = 0,53$Å - радиус первой боровской орбиты в атоме водорода.

О3.1-4.21

Оценить скорость мюона μ^-в мезоатоме с зарядом ядра $Z = 10$. Найти радиус атома.

4.

21. $v_\mu \approx \frac{Ze^2}{\hbar} = Z\alpha c = 2,3 \cdot 10^9$ cm/c; $r_\mu = \frac{m_e}{Z(m_\mu)_{\text{прив}}} r_1 \approx 2,8 \cdot 10^{-12}$c, где $\alpha = \frac{e^2}{\hbar c} = \frac{1}{137}$ - постоянная тонкой структуры.

О3.1-4.22

При переходе пиона π^-с $4f$-оболочки на $3d$-оболочку мезоатома с ядром фосфора ($Z = 15$) испускается рентгеновский квант с энергией $\mathscr{E} = 40$ кэВ. Определить массу пиона и радиус $3d$-оболочки.

4.

22. $\mu_\pi c^2 \approx 137$МВ, где $\mu_\pi = \frac{m_\pi m}{m_\pi + m_9} \approx m_\pi$ - приведенная масса мезоатома, m_π - масса пиона, m_q - масса ядра. $r_\pi \approx \frac{9m_e}{m_\pi Z} r_1 \approx 1,2 \cdot 10^{-11}$ см.

О3.1-4.23

Какова была бы энергия связи и радиус водородоподобной системы из двух нейтронов при учете только силы гравитационного притяжения между ними?

О3.1-4.24

Какой радиус имела бы $2p$-оболочка атома из нейтрона и электрона, связанных между собой только силой гравитационного взаимодействия?

О3.1-4.25

Найти потенциалы ионизации ионов He^+и Li^{++}.

О3.1-4.26

Определить наименьшую энергию, которую надо сообщить в основном состоянии трижды ионизованному атому бериллия, чтобы возбудить полный спектр этого атома.

О3.1-4.27

Энергия ионизации атома He равна 24,5 эВ. Определить энергию $\mathfrak{g}$, необходимую для получения из нейтрального атома He дважды ионизованного иона He^{++}.

О3.1-4.28

Ядро атома трития, находящееся в основном состоянии, испытывает β^--распад. Считая, что за время вылета распадного электрона состояние атомного электрона не успевает измениться, найти его полную энергию сразу после распада.

О3.1-4.29 Вклад сильного взаимодействия в разность уровней

В 1989 г. в ЦЕРНе при пропускании медленных антипротонов через водородную камеру наблюдалось образование протониума - атома состава ($p\bar{p}$). Энергия излучения, соответствующая переходу протониума из состояния $2p$ в $1s$, оказалась равной 10,1 кэВ. Определить вклад сильного взаимодействия в разность энергий указанных уровней. Для какого из этих уровней вклад сильного взаимодействия оказывается наибольшим?

Solution (???)

4.29*. Вклад сильного взаимодействия $\Delta\mathscr{E} = 0,7$ кэВ.

Решение. Прежде всего, определим энергию излучения протониума, определяемую исключительно кулоновским взаимодействием, возникающим между протоном p и антипротоном $\tilde{p}$. Связанная система ($\tilde{p}$) аналогична позитронию. Поэтому для расчета кулоновского взаимодействия можно использовать результат задачи 4.18 с заменой массы электрона на массу про тона. Это дает уровни энергии протониума

$$\mathscr{E}_n = -\frac{m_\text{p} e^4}{2\hbar^2 n^2} = -\,\text{Ry}\,\frac{m_\text{p}}{m_\text{e}}\frac{1}{2n^2} \approx -12,5\frac{1}{n^2}\ \text{кэВ}.$$

Следовательно, вклад кулоновского взаимодействия в энергию перехода $2p \to 1s$ в атоме протониума составляет

$$\Delta\mathscr{E}_\text{Ку} = 12,5\left(\frac{1}{1^2} - \frac{1}{2^2}\right) \approx 9,4\ \text{кэВ}.$$

Расхождение с экспериментальным значением обусловлено вкладом сильного взаимодействия. Таким образом,

$$\Delta\mathscr{E}_\text{сил} = \Delta\mathscr{E} - \Delta\mathscr{E}_\text{ку} = 10,1 - 9,4 \approx 0,7\ \text{кэВ}.$$

В силу короткодействия ядерных сил их влияние на положение $2p$-состояния незначительно по сравнению с $1s$-состоянием, поскольку в кулоновском потенциале вероятность частице в $2p$-состоянии попасть в окрестность начала координат близка к нулю.

О3.1-4.30

За счет сильного взаимодействия энергия основного состояния протониума (системы $(\text{p}\tilde{\text{p}})$) сдвигается на $\delta E = 0,7$ кэВ относительно его «чисто кулоновского» значения. Считая, что сильное взаимодействие описывается потенциалом Юкавы $U(r) = -\left(g^2/r\right)\exp\left(-r/r_0\right)$, $r_0 = 0,8\cdot 10^{-13}$см, оценить величину константы сильного взаимодействия $g^2/(\hbar c)$ (функция $1s$-состояния протониума $\psi = \left(\pi r_5^3\right)^{-1/2}\exp\left(-r/r_5\right)$, где r_b - боровский радиус протониума.

4.

30. $\frac{g^2}{\hbar_c} = \frac{r_\text{Б}^3\,|\delta\S|}{4\hbar c r_0^2} \approx 0,27$. Сравните с 10.59 и 10.60 .

Маг-МФТИ-вструп.5 возбужденные вращательные уровни в HCl

Оценить количество вращательных уровней молекулы HCl возбуждаемых при комнатной температуре (300K). Межъядерное расстояние у этой молекулы равно d=1.27 Å

Solution

масса HCl $= m_p + 35m_p$ из таблицы менделеева (наверное) ибо у водорода масса - масса протона, а хлор это 35 нуклонов.
Нужно
Энергия вращательного движения:

$$E_\text{вр} = \frac{\hbar^2 l(l+1)}{2\mu d^2}$$

(потом подумаю, как вывести её)
то есть нужно найти максимальное l
В то же время энергия квант тепловой энергии молекулы kT, на одну степень свободы приходится $1/2$ этой энергии. у нас две степени свободы, поэтому есть две половины kT, так что:

$$E_T = kT$$

сравниваем эти выражения.
высчитаем сперва поотдельности каждое, далее условие на l состоит в том, что оно максимальное, при котором энергия меньше возможной при данной температуре:

$$1.3l(l+1) < 25$$

для $l = 4$ это так.
(потом подоказываю, откуда вообще формулы эти)

О3.1-4.31

Фотон головной (наиболее длинноволновой) линии серии Лаймана иона гелия He^+поглощается водородным атомом в основном состоянии и ионизует его. Определить кинетическую энергию T, которую при этом получит электрон.

О3.1-4.32

Атом водорода, вначале находившийся в неподвижном состоянии, излучил квант света, соответствующий головной (наиболее длинноволновой) линии серии Лаймана. Определить относительное изменение частоты фотона $\Delta v/v_0$ из-за отдачи. Какую скорость приобрел атом за счет энергии отдачи?

SOLUTIONS 4. Атом водорода и водородоподобные атомы

4.

8. $\left\langle \frac{1}{r} \right\rangle = \frac{1}{r_I}$.

Примечание. Здесь можно обойтись без интегралов. Достаточно использовать теорему вириала для кулоновского поля

$$2\langle T\rangle = -\langle U\rangle, \text{ откуда:}$$
$$\mathscr{E}_n = \langle T\rangle + \langle U\rangle, \text{ и при } n = 1$$
$$\mathscr{E}_1 = -\frac{e^2}{2r_1} = -\frac{1}{2}\langle U\rangle = e^2\left\langle \frac{1}{r} \right\rangle.$$

Таким образом,

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{r_1}.$$

4.

9. $\langle U\rangle = -\frac{Ze^2}{r_1}; \langle T\rangle = \frac{Ze^2}{2r_1} = -\frac{\langle U\rangle}{2}$. (См. примечание к ответу задачи 4.8.)

4.

10. $\alpha = -\frac{me^2}{2\hbar^2}; \beta = \frac{me^2}{2\hbar^2}; \mathscr{E} = -\frac{me^4}{8\hbar^2}$, откуда $n = 2$.

Поскольку $\psi = \psi(r)$, то $l = 0$. Это $2s$ - состояние. Если $\alpha = 0$, то это основное состояние $1s$; при этом $\beta = \frac{1}{r_1} = \frac{me^2}{\hbar^2}; n = 1; \mathscr{E} = -\frac{me^4}{2\hbar^2}$. См. также решение задачи 3.10.

4.

11. $R > 2\frac{m_\text{н}}{m_\text{e}} \approx 3700; b > \frac{R}{dn/d\lambda} \approx 3,7$ см.

4.

12. Разрешающая способность должна быть не меньше $\frac{3}{2}\frac{m_\text{p}}{m_\text{e}} \approx 2800$. Она одинакова для всех линий спектральных серий смеси. Разрешающая способность призмы $b\frac{dn}{d\lambda} = 1000$, т. е. недостаточна для разрешения. Для интерферометра Фабри-Перо должны выполняться неравенства:

$$m < \frac{3}{2}\frac{m_\text{p}}{m_\text{e}} < N_\text{Эфф}\, m$$

4.

13. Требуемая разрешающая способность $\frac{\lambda}{\delta\lambda} = \frac{\omega}{\delta\omega} = \frac{2m_\text{p}}{m_\text{e}} \approx 3700$. Она одинакова для всех линий серии, $N > \frac{1}{2}\frac{\lambda}{\delta\lambda} \approx 1850$.

4.

14. $N \approx \frac{m^3}{8} \approx 3400$ штрихов.

4.

15. $d_{\min} = \frac{\lambda_{\text{H}}\lambda_{\text{D}}}{2(\lambda_{\text{D}}-\lambda_{\text{H}})}\frac{1}{n_{\text{e}}-n_{\text{o}}} \approx \frac{\lambda^2}{2\Delta\lambda}\frac{1}{n_{\text{e}}-n_{\text{o}}} = 13,24$ см, $\frac{\lambda}{\Delta\lambda} \simeq \frac{2m_{\text{p}}}{m_{\text{e}}} \approx 3700$.

4.

16. $L_{\min} = \frac{M_1M_2}{(M_2-M_I)m_{\text{e}}}\frac{\hbar c}{W}\frac{1-r}{\sqrt{r}} = 1,37$ см.

4.

17. $r_1 = \frac{\hbar^2}{e^2 m_\mu Z} \approx \frac{1}{Z}\cdot 0,0026\cdot 10^{-8}$ см, что примерно в 200 раз меньше соответствующего значения r_1 для водородоподобного иона с тем же значением заряда ядра Z. Результат получен в предположении, что K-орбита мюона проходит вне ядра. Электронная оболочка практически не оказывает влияния на этот результат, так как из-за сферической симметрии электронного облака создаваемое им электрическое поле в месте нахождения мюона считается равным нулю. В том же предположении

$$\mathscr{E}_n = -\frac{m_\mu e^4}{2\hbar^2}\frac{Z^2}{n^2} \approx -2810\frac{Z^2}{n^2} \ni \text{ В}$$

Отсюда видно, что излучение, возникающее при переходе мюона на K-орбиту с более высоких орбит, будет расположено в рентгеновской области спектра, а при больших Z - в области γ-лучей. При больших ZK-орбита мюона проходит внутри ядра атома. В этом случае приведенные выше формулы становятся неприменимыми. Результаты сильно зависят от распределения электрического заряда в ядре, с чем и связана возможность использования мезоатомов для изучения распределения электрического заряда в атомном ядре.

4.

18. $\mathscr{E}_n = -\frac{hc}{2n^2}R_\infty, \mathscr{E} = -\mathscr{E}_1 = \frac{hc}{2}R_\infty = 6,80 \ni$, $\lambda_{\text{рез}} = \frac{8}{3R_\infty} = 243,0045$ нм, где постоянная Ридберга $R_\infty = 109737,3$ см$^{-1}$.

4.

23. $|\mathscr{E}_1| = \frac{\gamma^2 m_{\text{n}}^2}{4\hbar^2} \sim 10^{-83}$ эрг; $r_1 = \frac{2\hbar^2}{\gamma m_{\text{n}}^3} \sim 10^{28}$с.

Размер «бинейтронного атома» так велик, что неучет действия других масс Вселенной, очевидно, совершенно недопустим.

4.

24. $r_n = n^2\frac{\hbar^2}{m_e^2\gamma m_{\text{n}}}; r_2 \approx 4\cdot 10^{31}$ см, где $n = 1, 2, 3, \ldots$ - главное квантовое число.

4.

25. $V_{\text{He}} = 4V_{\text{H}} = 54,4$ В; $V_{\text{Li}} = 9V_{\text{H}} = 122,4$ В.

4.

26. $\mathscr{E}_{\text{Be}} = Z^2 e V_{\text{H}} = 217,6$ эВ.

4.

27. $\mathscr{E} = 78,9$ эВ.

4.

28. $\langle \delta_2 \rangle = \langle T \rangle + \langle U_2 \rangle = -40,8$ эВ, где $\langle T \rangle = 13,6$ эВ, $\langle U_2 \rangle = -\left\langle \frac{2e^2}{r} \right\rangle = -\frac{2e^2}{r_{\text{S}}} = -54,4$ эВ. Здесь усреднение идет по волновой функции атома трития.

4.

31. $T = 2\mathscr{E}_{\mathbf{n}} = 27,2$ эВ, где $\mathscr{E}_{\mathbf{n}}$ - энергия ионизации атома водорода.

4.

32. $\frac{\nu_0 - v}{v_0} = \frac{h\nu_0}{2m_{\text{a}}c^2} = \frac{3}{16}\frac{m_{\text{e}}}{m_{\text{at}}}\alpha^2 = 5,44 \cdot 10^{-9}$; $v = \frac{3}{8}\frac{m_{\text{e}}}{m_{\text{at}}}\alpha^2 c = 326$ cm/c, где $\alpha = e^2/\hbar c = 1/137$ - постоянная тонкой структуры.

4.

33. Водородная лампа должна удаляться от дейтериевой со скоростью $v \approx 82$ km/c.

4.

34. Угол конуса разлета γ-квантов отличается от развернутого на $\alpha \approx 1,2 \cdot 10^{-2}$ рад.

4.

35. $v_e = v_{\tilde{e}} = \frac{e^2}{2\sqrt{2}\hbar} \approx 8 \cdot 10^7$ cm/c (угол разлета $\approx 180°$).

4.

36. $\Delta\varphi = \frac{m_e e^2 \lambda}{4\pi\hbar^2} \approx 0,15$ рад $\approx 10°$.

Решение. Разброс в углах разлета электронов происходит из-за наличия перпендикулярно направленной импульсу фотона составляющей импульса электрона; ее наличие связано с движением электронов в атоме. Полный импульс электрона $p = \sqrt{p_\parallel^2 + p_\perp^2}$.

Перпендикулярную составляющую $p_\perp$, обеспечивающую максимальное отклонение, легко оценить из сооотношения неопределенностей:

$$\Delta p \Delta r \sim \hbar, \quad \text{где} \quad \Delta p \approx p_\perp, \quad \Delta r = r_1 = \frac{\hbar^2}{me^2}$$

Таким образом,

$$p_\perp \approx \frac{me^2}{\hbar} = m\alpha c$$

где $\alpha = e^2/\hbar c$ - постоянная тонкой структуры. Для нахождения составляющей импульса $p_\parallel$, направленной вдоль движения электрона, достаточно написать закон сохранения импульса:

$$\frac{h}{\lambda} = p_\parallel - \frac{h}{\lambda + \delta\lambda}$$

Величина комптоновского смещения $\delta\lambda$ определяется по известной формуле

$$\delta\lambda = 4\pi\Lambda_\mathrm{e} \approx 0,0485\text{Å} \ll \lambda = 1\text{Å}$$

Таким образом,

$$p_\parallel \approx \frac{2h}{\lambda}$$

Максимальный угол отклонения электрона

$$\operatorname{tg}\varphi = \frac{p_\perp}{p_\parallel} \approx \frac{mc\alpha}{2h/\lambda} = \frac{me^2\lambda}{4\pi\hbar^2} = 0,15, \quad \text{т. е.} \quad \varphi \approx 0,15 \text{ рад } \approx 8,6^\circ$$

Заметим, что для получения ответа можно было бы воспользоваться и законом сохранения энергии.

$$\frac{hc}{\lambda} + \mathscr{E} = \frac{hc}{\lambda + \delta\lambda} + \sqrt{m^2c^4 + p^2c^2}$$

Энергия электрона $\mathscr{E}_{9\mathbf{\Omega}} = mc^2 - |\mathscr{E}_\mathrm{CB}|$. Для водорода очевидно, что $|_{\text{св}}| \ll mc^2$, т. е. $\mathscr{G}_{9\Omega} \approx mc^2$. Энергия рентгеновского кванта $hc/\lambda = 12,4$ кэВ. Поэтому

$$mc^2 \gg \frac{hc}{\lambda} \gg |\mathscr{E}_\mathrm{CB}|$$

Кроме того, $p_\perp \ll p_\parallel$, что выясняется простым подсчетом. Поэтому

$$\sqrt{m^2c^4 + p^2c^2} \approx \sqrt{m^2c^4 + p_\parallel^2c^2} \approx mc^2 + \frac{p_\parallel^2}{2m}.$$

Подставив все это в закон сохранения энергии, получим

$$\frac{hc}{\lambda} \approx \frac{hc}{\lambda + \delta\lambda} + \frac{p_\parallel^2}{2m}, \text{ откуда } p_\parallel \approx \sqrt{\frac{2mhc\delta\lambda}{\lambda^2}} = \frac{2h}{\lambda}, \text{ где } \delta\lambda = \frac{2h}{mc}.$$

4.

37. $\Delta\varphi = \frac{Zm_\mathrm{e}e^2\lambda}{2\pi\hbar^2} \approx 0,25$ рад $\approx 14^\circ$.

4.

38: $T_\mathrm{e} = 10,2$ кэВ.

Решение. Согласно закону Мозли энергия кванта, излученного при переходе электрона с уровня n_2 на уровень n_1 (заряд ядра Z, а σ - поправка на экранирование заряда ядра электронами K-оболочки)

$$\mathscr{E} = \hbar\omega = \mathrm{Ry}(Z - \sigma)^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right).$$

Для линии $K_\alpha n_1 = 1, n_2 = 2$. Поскольку энергия такого кванта в спектре излучения серебра известна и равна $\mathscr{E} = 21,6$ кэВ, то из приведенной формулы найдем поправку σ на экранирование заряда ядра электронами на K-оболочке (в обоих случаях $Z < 50$)

$$\sigma = Z_\mathrm{Ag} - \sqrt{\frac{4\mathscr{E}}{3\mathrm{Ry}}} \approx 1$$

Энергия, необходимая для освобождения электрона из K-оболочки атома $_3$Zn (переход с $n = 1$ в $n = \infty$), равна

$$(\hbar\omega)_\mathrm{Zn} = \mathrm{Ry}\left(Z_{Z\mathrm{n}} - 1\right)^2 = 13,6 \cdot 29^2 = 11,4\text{k B}B,$$

а значит, кинетическая энергия T_e вылетевшего оттуда электрона равна

$$T_\mathrm{e} = \mathscr{E} - (\hbar\omega)_\mathrm{Zn} = 21,6 - 11,4 = 10,2\kappa \text{ B}.$$

4.

39. Отличие в $n^4 = 10^4$ раз.

18.1.6 Basic Problems about Hydrogen Atoms 2

O3.1-4.33

С какой скоростью и в каком направ.ении должна двигаться светящаяся газоразрядная лампа, заполненная водородом, чтобы в ней происходило поглощение света, излучаемого неподвижной газоразрядной лампой, заполненной дейтерием? Рассмотреть движение вдоль прямой, соединяющей лампы.

O3.1-4.34

При аннигиляции позитронов с электронами образуются два γ-кванта, уносящие энергию покоя аннигилировавших частиц. Если бы электрон и позитрон перед аннигиляцией покоились, γ - кванты разлетались бы в строго противоположных направлениях. В реальном процессе аннигиляции замедленные в веществе позитроны сталкиваются с движущимися атомными электронами, и угол конуса разлета η-квантов отличается от 180°. Оценить, насколько этот угол отличается от развернутого, если аннигиляция происходит на электронах L-оболочки углерода.

O3.1-4.35

Позитроний поглощает фотон, образовавшийся при переходе атомарного водорода из первого возбужденного состояния в основное. Определить скорости электрона и позитрона в случае их симметричного относительно направления движения фотона разлета. Атом в исходном состоянии считать неподвижным.

O3.1-4.36

При комптоновском рассеянии квантов на атомных электронах явление осложняется тем, что электроны в атомах не находятся в покое. Оценить связанный с этим разброс в углах разлета электронов отдачи, выбиваемых из атомов водорода при рассеянии рентгеновских квантов ($\lambda = 1$Å) строго назад.

O3.1-4.37

Решить предыдущую задачу для электронов отдачи, выбиваемых с K-оботочки атомов свинца при рассеянии гамма-квантов с д.иной волны $\lambda = 0,01$Å строго назад. Для свинца $Z = 82$.

O3.1-4.38

Считая, что поправка на экранирование заряда ядра электронами на K-оболочке одинакова для атомов с $Z < 50$, найти кинетическую энергию T_e фотоэлектронов, вылетающих из K-оболочки атомов ${}_{30}$Zn под действием K_α-излучения серебра ${}_{47}$Ag с энергией 21,6 кэВ.

O3.1-4.39

Во сколько раз отличаются средние длины свободного пробега атома водорода в основном и возбужденном состояниях ($n = 10$) в разреженном одноатомном газе при одинаковой концентрации?

O3.1-4.40

В электрическом поле возможна спонтанная ионизация атомов. Оценить, при какой величине напряженности поля E (в В/см) окажется ионизованным атом водорода в состоянии с $n = 10$. Энергии уровней считать не зависящими от поля.

4.

40. $E = \frac{\text{Ry}^2}{4e^3 n^4} \approx 32$ КВ/cm.

O3.1-4.41

Задача об отыскании уровней энергии атомов обычно решается в предположении, что заряд ядра точечный. На самом деле ядро имеет размер, и радиусы ядер $R_{\text{я}} = 1,3 \cdot 10^{-13} A^{1/3}$см, где A - атомная масса. Определить знак и оценить порядок величины относительной поправки $\Delta\mathscr{E}/\mathcal{E}$ к энергии мюона на K-оболочке в мезоатоме неона ($Z = 10, A = 20$), связанной с тем, что часть времени мюон находится внутри ядра, т. е. в поле с потенциалом, отличным от Ze^2/r. Волновая функция основного состояния электрона в атоме водорода $\psi = \frac{1}{\sqrt{\pi r_1^3}} e^{-r/r_t}$, где r_1 - радиус первой боровской орбиты. Масса мюона $m_\mu = 207 m_{\text{e}}$

4.

41: $\frac{\Delta\mathscr{G}}{\mathscr{G}} = \begin{cases} \frac{4}{3}\left(\frac{R_g}{r_{\mu 1}}\right)^2 = 2,53 \cdot 10^{-2} \text{ (ядро - заряженная сфера)}, \\ \frac{4}{5}\left(\frac{R_g}{r_{\mu 1}}\right)^2 = 1,52 \cdot 10^{-2} \text{ (ядро - однородно заряженный шар)}, \end{cases}$ где $r_{\mu 1} = \frac{\hbar^2}{m_\mu Z e^2}$.

Решение. Считаем, что решение задачи об уровнях энергии в кулоновском поле точечного заряда известно: $\widehat{H}\varphi = \delta \downarrow$, где $\widehat{H} = \frac{\hat{p}^2}{2m} - \frac{Ze^2}{r}$,

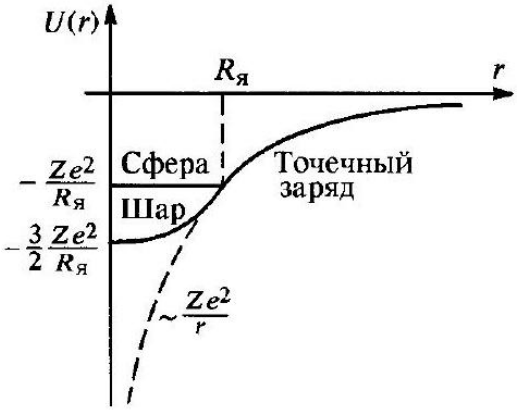


Рис. 154

$\mathscr{E} = -\frac{z^2 m e^4}{2\hbar^2}\frac{1}{n^2}$. Рассмотрим $n = 1$, тогда $\psi_1 = \frac{1}{\sqrt{\pi r_1^3}} e^{-r/r_1}$. Истинный потенциал при $r \geqslant R_{\text{я}}$ совпадает с потенциалом точечного ядра и отличается от него при $r < R_{\text{я}}$. Если считать ядро равномерно заряженной по поверхности сферой, то $U(r < R_{\text{q}}) = -\frac{Ze^2}{R_{\text{я}}}$; если равномерно заряженным шаром, то $U(r < R_{\text{g}}) = -\frac{3}{2}\frac{Ze^2}{R_{\text{я}}}\left(1 - \frac{r^2}{3R_q^2}\right)$, (рис. 154).

Представим истинный гамильтониан в виде

$$\widehat{H} = \frac{\hat{p}^2}{2m} - \frac{Ze^2}{r} + \delta U,$$

где для шара

$$\delta U = \begin{cases} 0, & r \geqslant R_{\text{g}}, \\ \frac{Ze^2}{r} - \frac{3}{2}\frac{Ze^2}{R_{\text{g}}}\left(1 - \frac{r^2}{3R_{\text{g}}^2}\right), & r < R_{\text{g}} \end{cases}$$

и для сферы

$$\delta U = \begin{cases} 0, & r \geqslant R_{\text{g}}, \\ \frac{Ze^2}{r} - \frac{Ze^2}{R_{\text{g}}}, & r < R_{\text{q}}. \end{cases}$$

Так как все отличие проис ходит при $r < R_{\text{g}} \ll r_1$, то рассматриваем δU как поправку. Среднее значение δU в основном состоянии и есть сдвиг уровня:

$$\langle\Psi_1|\,\hat{H}\,|\Psi_1\rangle = \langle\Psi_1|\,\frac{\hat{p}^2}{2m} - \frac{Ze^2}{r}\,|\psi_1\rangle + \langle\psi_1|\,\delta U\,|\psi_1\rangle = -\frac{mZ^2e^4}{2\hbar^2} + \Delta\mathscr{E},$$

$$\Delta\mathscr{E} = \int dV \Psi_1^* \delta U \psi_1 = \frac{1}{\pi r_1^3} 4\pi \int_0^{R_{\text{s}}} e^{-2r/r_1} \left\{ \begin{array}{c} \frac{Ze^2}{r} - \frac{Ze^2}{R_g} \\ \frac{Ze^2}{r} - \frac{3}{2}\frac{Ze^2}{R_g}\left(1 - \frac{r^2}{3R_{\text{A}}^2}\right) \end{array} \right) r^2 dr,$$

т. к. $\frac{R_9}{r_1} \leqslant \frac{3{,}5 \cdot 10^{-13}}{25{,}6 \cdot 10^{-13}} \sim 0,1$, то $e^{-2r/r_1} \simeq 1$. Тогда

$$\Delta\mathscr{E} \approx \frac{4}{r_1^3}\int_0^{R_g}\left\{\begin{array}{c} Ze^2\left(r-\frac{r^2}{R_g}\right) \\ Ze^2\left[r-\frac{3}{2}\frac{r^2}{R}\left(1-\frac{r^2}{3R_g^2}\right)\right]\end{array}\right\}dr = \left\{\begin{array}{l} \frac{2}{3}\frac{Ze^2}{r_1}\left(\frac{R_g}{r_1}\right)^2 - \text{ сфера}, \\ \frac{2}{5}\frac{Ze^2}{r_1}\left(\frac{R_g}{r_1}\right)^2 - \text{ шар.}\end{array}\right.$$

Видно, что поправка положительна, следовательно, уровни сдвигаются вверх. Относительная поправка

$$\delta = \left|\frac{\Delta\mathscr{E}}{\mathscr{Q}_1}\right| = \frac{\Delta\mathscr{E}}{\frac{Ze^2}{2r_1}} = \begin{cases}\frac{4}{3}\left(\frac{R_{\text{g}}}{r_1}\right)^2 & \text{- сфера} \\ \frac{4}{5}\left(\frac{R_{\text{f}}}{r_1}\right)^2 & \text{- шар.}\end{cases}$$

Сделаем вычисления:

$$R_{\text{g}} = 3,53\cdot 10^{-13}\text{c}, r_1 = r_{\mu_1} = \frac{\hbar^2}{m_\mu Ze^2} = \frac{m_{\text{e}}}{m_\mu}\frac{1}{Z}\frac{\hbar^2}{m_{\text{e}}e^2} = 25,6\cdot 10^{-13}\text{c}$$

$$\frac{\Delta\mathscr{E}}{\mathscr{E}} = \left\{\begin{array}{l} 2,53\cdot 10^{-2} - \text{ сфера} \\ 1,52\cdot 10^{-2} - \text{ шар.}\end{array}\right.$$

(остальное скорее всего порешаю потом, итак порешать бы это!)

там много еще хороших задач есть.

4.

42. $\frac{\Delta\mathscr{E}}{\mathscr{G}} = \left\{\begin{array}{l} \frac{4}{3}\left(\frac{R_{\text{Я}}}{a_{\text{Ne}}}\right)^2 = 5,94\cdot 10^{-7} \text{ (ядро - заряженная сфера)}, \\ \frac{4}{5}\left(\frac{R_{\text{я}}}{a_{\text{Ne}}}\right)^2 = 3,56\cdot 10^{-7} \text{ (ядро - однородно заряженный шар)}, \end{array}\right.$ где $a_{\text{Ne}} = \frac{r_1}{Z}$.

4.

43. $\langle T\rangle = \frac{e^2}{2r_1^*} \approx 14,5$ эВ, где $r_1^* = \frac{\hbar^2}{\mu e^2} \approx 0,5\cdot 10^{-8}$ см.

4.

44. $\langle T\rangle = \frac{e^2}{8r_1^*} \approx 3,4$ эВ, где $r_1^* = \frac{\hbar^2}{\mu e^2} \approx 0,5\cdot 10^{-8}$ см.

4.

45. Так как радиус мюонной орбиты $r_\mu = \frac{\hbar^2}{Ze^2 m_\mu} \approx 10^{-11}$ см $\ll r_{\text{Б}}$ - боровского радиуса $(0,53\text{Å})$, то оставшийся электрон фактически движется в поле с зарядом $Z = 1$ (водородоподобный атом). Энергия перехода между уровнями $n = 3$ и $n = 2$ равна (это линия H_α)

$$\frac{1}{\lambda_{32}} = R_\infty\left(\frac{1}{2^2}-\frac{1}{3^2}\right) = \frac{5}{36}R_\infty \approx 1,52\cdot 10^4 \text{ см}^{-1}; \quad \lambda_{32} = 656\text{НМ},$$

где $R_\infty = 109737,3$ см$^{-1}$.

4.

46. Энергия $3p$-состояния находится из условия $\mathscr{E}_{3p} = \mathscr{E}_{3s} + \frac{hc}{\lambda} = -U_0 + \frac{hc}{\lambda} = -3,0$ эВ. Поскольку $\mathscr{E}_{3\text{р}} = -\text{Ry}\frac{Z_{\text{эфф}}^2}{3^2}$, то получаем $Z^2 \approx 2$; $Z_{\text{Эфф}} \approx 1,4$.

4.

47. $v = \frac{3}{4}\frac{z^2 a}{h} Ry = 9 \cdot 10^8$ cm/c.

4.

48: $\mathscr{E}_{\text{осн}} \approx -\frac{e^2}{r} Z\left(Z - \frac{5}{8}\right) = -74,8$ эВ; где обозначено $r = \frac{\hbar^2}{m_e e^2} = 0,529\text{Å}$; $\varrho_{\text{ион}} \approx \frac{m e^4}{2\hbar^2} Z\left(Z - \frac{5}{4}\right) \approx 20,4$ эВ, где $Z = 2$.

Решение. Вычислим энергию кулоновского расталкивания электронов в атоме гелия. Это интеграл

$$\mathscr{E}_{\text{кул}} = e^2 \iint_0^\infty \psi^*(r_1, r_2) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \psi(r_1, r_2)\, d\mathbf{r}_1 d\mathbf{r}_2 =$$
$$= e^2 \int_0^\infty \int_0^\infty |\psi_0(\mathbf{r}_1)|^2 \cdot |\psi_0(\mathbf{r}_2)|^2 \frac{d\mathbf{r}_1 d\mathbf{r}_2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

Введем плотности зарядов

$$\rho(\mathbf{r}_1) = e\,|\psi_0(\mathbf{r}_1)|^2 \quad \text{и} \quad \rho(\mathbf{r}_2) = e\,|\psi_0(\mathbf{r}_2)|^2$$

Тогда

$$\mathfrak{E}_{\text{куп}} = 2 \cdot \frac{1}{2} \int_0^\infty \int_0^\infty \frac{\rho(\mathbf{r}_1)\,\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2 = 2 \cdot \frac{1}{2} \int_0^\infty \rho(\mathbf{r}_1)\,\varphi(\mathbf{r}_1)\, d\mathbf{r}_1$$

где $\varphi(\mathbf{r}_1) = \int_0^\infty \frac{\rho(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_2$ - потенциал, создаваемый в точке $\mathbf{r}_1$ распределением заряда $\rho(\mathbf{r}_2)$ - аналог формулы $\frac{1}{2}\sum_i q_i \varphi_i$ (в силу симметрии можно было бы написать $\mathscr{E}_{\text{кул}} = 2 \cdot \frac{1}{2}\int_0^\infty \rho(r_2)\,\varphi(r_2)\, dr_2$).

$$\varphi(\mathbf{r}_1) = \int_0^\infty \frac{\rho(r_2)\, 4\pi r_2^2 dr_2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

Разобьем область интегрирования на две части $\int_0^\infty = \int_0^{r_1} + \int_{r_1}^\infty$. Тогда первый интеграл есть потенциал, создаваемый сферически симметричным распределением заряда при $r_2 < r_1$. По теореме Гаусса он равен потенциалу точечного заряда, находящегося в центре сферы. То есть

$$\int_0^{r_1} \frac{\rho(r_2)\, 4\pi r_2^2 dr}{|\mathbf{r}_1 - \mathbf{r}_2|} = \frac{1}{r_1}\int_0^{r_1} \rho(\mathbf{r}_2)\, 4\pi r_2^2 dr = \frac{4Z^3}{r_{\text{B}}^3}\frac{e}{r_1}\int_0^{r_1} \exp\left(-\frac{2Zr_2}{r_{\text{B}}}\right) r_2^2 dr_2 =$$
$$= \frac{4e}{r_1}\left(\frac{Z}{r_{\text{E}}}\right)^3 \exp\left[-\frac{r_2^2 r_{\text{B}}}{2Z} - \frac{2r_2 r_{\text{B}}^2}{(2Z)^2} - \frac{2r_{\text{B}}^3}{(2Z)^3}\right] \exp\left(-\frac{2Zr_2}{r_{\text{E}}}\right)\Bigg|_0^{r_1} =$$
$$= 4e\left(\frac{Z}{r_{\text{E}}}\right)^3 \frac{(-1)}{r_1}\left\{\left[\frac{r_1^2 r_{\text{E}}}{2Z} + \frac{r_1 r_{\text{F}}^2}{4Z^2} + \frac{r_{\text{E}}^3}{8Z^3}\right]\exp\left(-\frac{2Zr_1}{r_{\text{B}}}\right) - \frac{r_{\text{B}}^3}{8Z^3}\right\} =$$
$$= -4e\left\{\left[\frac{r_1 Z^2}{2r_{\text{Б}}^2} + \frac{Z}{4r_{\text{Б}}} + \frac{1}{8r_1}\right]\exp\left(-\frac{2Zr_1}{r_{\text{Б}}}\right) - \frac{1}{8}\frac{1}{r_1}\right\}$$

Для вычисления поля, создаваемого распределением заряда при $r_2 > r_1$, разбиваем всю область на вложенные друг в друга сферы толщиной dr с зарядом $dQ = \rho(r_2) \cdot 4\pi r_2^2 dr_2$ (рис. 155).

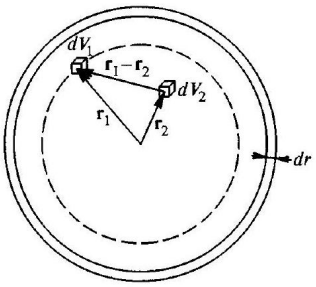


Рис. 155

По теореме Гаусса потенциал внутри сферы равен потенциалу ее поверхности. Таким образом, $\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \to \frac{1}{r_2}$

$$\int_{r_1}^{\mathrm{U}} \to \int_{r_1}^{\infty} \frac{\rho(r_2)\,4\pi r_2^2 dr_2}{r_2} = 4\left(\frac{Z}{r_{\mathrm{E}}}\right)^3 e \int_{r_1}^{\infty} \exp\left(-\frac{2Z}{r_{\mathrm{E}}} r_2\right) r_2 dr_2 =$$
$$= 4\left(\frac{Z}{r_{\mathrm{E}}}\right)^3 e \cdot \exp\left(-\frac{2Z}{r_{\mathrm{E}}} r_2\right) \frac{r_{\mathrm{E}}^2}{(2Z)^2} \left(-\frac{2Z}{r_{\mathrm{E}}} \cdot r_2 - 1\right)_{r_1}^{\infty} =$$
$$= \left(\frac{Z}{r_{\mathrm{E}}}\right)^3 \cdot e \cdot \exp\left(-\frac{2Z}{r_{\mathrm{E}}} r_1\right) \left(\frac{r_{\mathrm{B}}}{Z}\right)^2 \left(2\frac{Z}{r_{\mathrm{E}}} r_1 + 1\right) =$$

$$= \frac{Z}{r_{\mathrm{E}}} \cdot e \cdot \exp\left(-\frac{2Z}{r_{\mathrm{E}}} r_1\right) \left(2\frac{Z}{r_{\mathrm{E}}} r_1 + 1\right).$$

Складывая, получаем

$$\varphi(r_1) = \frac{e}{r_1} - e\left(\frac{Z}{r_{\mathrm{B}}} + \frac{1}{r_1}\right) \exp\left(-\frac{2Z}{r_{\mathrm{B}}} r_1\right)$$

Тогда

$$\mathscr{E}_{\text{ку.}} = \int_0^{\infty} \rho(\boldsymbol{r}_1)\,\varphi(r_1)\,dr_1 = \frac{4\pi Z^3}{\pi r_{\mathrm{B}}^3} e^2 \int_0^{\infty} \exp\left(-\frac{2Z}{r_{\mathrm{Б}}} r_1\right) \times$$
$$\times \left\{\frac{1}{r_1} - \left(\frac{Z}{r_{\mathrm{G}}} + \frac{1}{r_1}\right) \exp\left(-\frac{2Z}{r_{\mathrm{E}}} r_1\right)\right\} r_1^2 dr_1 =$$
$$= 4\left(\frac{Z}{r_{\mathrm{E}}}\right)^3 e^2 \left\{\int_0^{\infty} \exp\left(-\frac{2Z r_1}{r_{\mathrm{E}}} r_1\right) dr_1 -\right.$$
$$\left. -\frac{Z}{r_{\mathrm{E}}} \int_0^{\infty} \exp\left(-\frac{4Z}{r_{\mathrm{E}}} r_1\right) r_1^2 dr_1 - \int_0^{\infty} \exp\left(-\frac{4Z}{r_{\mathrm{E}}} r_1\right) r_1 dr_1 \right\} =$$
$$= 4\left(\frac{Z}{r_{\mathrm{B}}}\right)^3 e^2 \left\{\left(\frac{r_{\mathrm{B}}}{2Z}\right)^2 \int_0^{\infty} e^{-y' y dy - \frac{Z}{r_{\mathrm{B}}}\left(\frac{r_{\mathrm{B}}}{4Z}\right)^3 \int_0^{\infty} e^{-y^2} y^2 dy - \left(\frac{r_{\mathrm{B}}}{4Z}\right)^2 \int_0^{\infty} e^{-y} y dy}\right\} \ldots$$

Так как $\int_0^{\infty} e^{-y} y^n dy = \Gamma(n+1) = n!$, то

$$\mathring{\mathrm{A}}_{\text{ку}} = 4e^2 \left(\frac{Z}{r_{\mathrm{B}}}\right)^3 \left\{\left(\frac{r_{\mathrm{B}}}{2Z}\right)^2 \cdot 1! - \frac{1}{4^3}\left(\frac{r_{\mathrm{B}}}{Z}\right)^2 \cdot 2! - \frac{r_{\mathrm{B}}}{4^2 Z^2} \cdot 1!\right\} =$$
$$= 4e^2 \frac{Z}{r_{\mathrm{E}}} \left\{\frac{1}{4} - \frac{2}{64} - \frac{1}{16}\right\} = 4e^2 \frac{Z}{r_{\mathrm{B}}} \frac{16 - 2 - 4}{64} = \frac{5}{8} \frac{Z e^2}{r_{\mathrm{B}}},$$
$$\mathscr{E}_{\text{осн}} = -2\mathrm{Ry} + \mathrm{E}_{\text{кул}} = -2\frac{Z^2 e^2}{2r_{\mathrm{E}}} + \frac{5}{8}\frac{Z}{r_{\mathrm{B}}} = -Z\left(Z - \frac{5}{8}\right)\frac{e^2}{r_{\mathrm{D}}} = -74{,}8 \text{ В}.$$

После ионизации, т.е. отрыва одного электрона, останется водородоподобный ион с зарядом $+2$. Энергия связи оставшегося электрона есть

$$\mathscr{E}_{\text{СВ}} = -Z^2 \mathrm{Ry} = -Z^2 \frac{e^2}{2r_{\mathrm{B}}}$$
$$\mathscr{E}_{\text{ион}} = \mathscr{E}_{\text{СВ}} - \mathscr{E}_{\text{ОСН}} = Z\left(Z - \frac{5}{8}\right)\frac{e^2}{r_{\mathrm{B}}} - Z^2 \frac{e^2}{2r_{\mathrm{B}}} = Z\left(Z - \frac{5}{4}\right)\frac{e^2}{2r_{\mathrm{B}}} = 20{,}4 \ni \text{ В}$$

4.

49. $3d$-состояние.

4.

50. $2s$-состояние.

4.

51*. $\lambda'' = 3,7$ нм; $T = mc^2\left(\frac{1}{\sqrt{1-v^2/c^2}} - 1\right) \approx 11,6$ ГэВ.

Решение. Частота лазерного излучения в ЛСО $\omega_0 = 2\pi c/\lambda_0$. В системе отсчета ионов (где они неподвижны) эта же частота

$$\omega' = \omega_0\sqrt{\frac{1+\beta}{1-\beta}},\ \text{где}\ \beta = \frac{v}{c}$$

Энергия перехода иона гелия из основного состояния в первое возбужденное $\mathscr{E}_{12} = \text{Ry}\ Z^2\left(\frac{1}{1^2} - \frac{1}{2^2}\right) = 3\text{Ry} = \hbar\omega'$. Поскольку $\frac{\left(\hbar\omega'\right)^2}{(\hbar\omega)^2} = \frac{1+\beta}{1-\beta}$, то $\beta = \frac{(\mathscr{E}_{12}/\hbar\omega_0)^2-1}{(\mathscr{E}_{12}/\hbar\omega_0)^2+1} \approx 0,97$. Здесь $\hbar\omega_0 = \frac{2\pi c\hbar}{\lambda_0} = 5$ эВ .

Частота излучения в ЛСО (см. задачу 1.35)

$$\omega'' = \omega'\sqrt{\frac{1+\beta}{1-\beta}} = \omega_0\frac{1+\beta}{1-\beta} = \left(\frac{\mathscr{E}_{12}}{\hbar\omega_0}\right)^2\omega_0 \approx 66,6\omega_0$$

Эта частота соответствует длине волны

$$\lambda'' = \frac{\lambda_0}{66,6} \approx 3,7\text{НМ}$$

Кинетическая энергия ионов

$$T = mc^2\left(\frac{1}{\sqrt{1-\beta^2}} - 1\right) \approx 11,6\Gamma\ni\ \text{В}$$

4.

52. $\tau \simeq \frac{\hbar\omega}{I} = \frac{3}{2}\frac{Z^2}{n^4}\alpha\hbar\frac{\left(mc^2\right)^2}{(\hbar\omega)^3} = 6,6\cdot 10^{-12}$с, где $\hbar\omega = \frac{3}{4}\text{Ry}Z^2 = 40,8$ В, $Z = 2, n = 2, \alpha = \frac{e^2}{\hbar c} = \frac{1}{137}$.

4.

53. $\text{t} \simeq \frac{\hbar\omega}{I} = \frac{3}{2}\frac{Z^2}{n^4}\alpha\hbar\frac{\left(mc^2\right)^2}{(\hbar\omega)^3} = 0,2\cdot 10^{-7}$с, где $\hbar\omega = \text{Ry}\ Z^2\left(\frac{1}{9^2} - \frac{1}{10^2}\right) = 0,51\rho$ В.

4.

54. $\left(\frac{\Delta\mathscr{E}}{\mathscr{E}}\right)_{\text{Pb}} = \left(\frac{\Delta\mathscr{E}}{\mathscr{E}}\right)_{\text{Ne}}\frac{\left(Z^2R_{\text{я}}^2\right)_{\text{Pb}}}{\left(Z^2R_{\text{яд}}^2\right)_{\text{Ne}}} = 1,92\cdot 10^{-4}$.

4.

55. $R \leqslant 512\frac{\gamma M}{c^2}\left(\frac{Br_1^2}{e}\right)^2 \simeq 6500$ км, где $r_1 = \frac{\hbar^2}{m_e e^2} = \frac{e^2}{2\text{Ry}} \approx 0,53\text{Å} - 60$ - ровский радиус (см. задачу 4.40).

18.1.7 Advanced problems about atoms 1

ГК-5.1 Минимизация

Используя неравенство

$$\int |\nabla\psi + Z\psi\nabla r|^2 d\tau \geqslant 0,$$

найти минимальную энергию одноэлектронного атома и соответствующую этой энергии волновую функцию. Показать, что для основного состояния атома выполняется соотношение $2\bar{T} \geqslant |\bar{v}|$.

ГК-5.2 Средний электростатический потенциал

Электрон в кулоновом поле ядра заряда Z находится в основном состоянии. Показать, что средний электростатический потенциал в пространстве, создаваемый ядром и электроном, равен

$$\varphi = \frac{e(Z-1)}{r} + e\left(\frac{Z}{a} + \frac{1}{r}\right)e^{-\frac{2Zr}{a}}, \quad \left(a = \frac{\hbar^2}{\mu e^2}\right).$$

ГК-5.3 Свойства радиуса орбиты

3. Показать, что в основном состоянии атома водорода:
а) наивероятное значение r равно $a = \frac{\hbar^2}{\mu \cdot e^2}$,
б) среднее значение $\frac{\overline{1}}{r} = \frac{1}{a}$,
в) $\frac{\overline{1}}{r^2} = \frac{2}{a^2}$.

ГК-5.4 Плотность вероятности протона

Волновая функция $\psi(\boldsymbol{r})$ описывает относительное движение двух частиц: протона и электрона. Пусть координаты центра масс атома водорода точно известны и равны

$$X = 0, \quad Y = 0, \quad Z = 0.$$

Показать, что в этом случае плотность вероятности для протона имеет вид

$$w(\boldsymbol{r}) = \left(\frac{m+M}{m}\right)^3 |\psi\left(\frac{m+M}{m}\boldsymbol{r}\right)|^2,$$

где m и M-массы электрона и протона соответственно.

ГК-5.5. Распределение по импульсам

Найти распределение по импульсам электрона в атоме водорода для состояний $1s, 2s$ и $2p$.

ГК-5.6. Среднее квадратичное отклонение расстояния

Вычислить $\overline{r^2} - \bar{r}^2$ среднее квадратичное отклонение расстояния электрона от ядра для электрона в атоме водорода, находящегося в состоянии с квантовыми числами n, l.

ГК-5.7.

Выразить собственную волновую функцию атома водорода в параболических координатах с $n_1 = 1, n_2 = 0$, $m = 0$ через волновые функции в сферических координатах. Показать также, что

$$\psi_{n_1=0,n_2=0,m=n-1}(\xi, \gamma_i, \varphi) = \psi_{n,l=n-1,m=n-1}(r, \vartheta, \varphi).$$

ГК-5.8.

Показать непосредственно, что степень вырождения n-го собственного значения энергии атома водорода при решении уравнения Шредингера в параболических координатах равняется n^2.

ГК-5.9.

Найти поправку к уровням энергии атома водорода за счет релятивистской зависимости массы от скорости (учесть член порядка $\frac{v^2}{c^2}\Big)$.

ГК-5.10.

Из релятивистского уравнения для электрона (уравнения Дирака) следует, что, кроме поправки, учитывающей зависимость массы от скорости $\left(\sim \frac{v^2}{c^2}\right)$, существует еше один член в гамильтониане

$$H_2 = \frac{\hbar^2}{2\mu\mu^2 c^2}\frac{1}{r}\frac{dU}{dr}\hat{\boldsymbol{l}}\hat{\boldsymbol{s}},$$

где $\hat{\boldsymbol{i}}$ - оператор орбитального момента, $\hat{\boldsymbol{s}}$ - оператор спина, $U(r)$ - потенциальная энергия электрона (потенциал предполагается центрально-симметричным). Наглядный смысл этого члена заключается в том, что при движении магнитного момента $\boldsymbol{\mu}$ (связанного со спином электрона) появляется дипольный электрический момент $\boldsymbol{d} = \frac{1}{c}$ [?p], который взаимодействует с полем ядра. Найти поправку к уровням энергии атома водорода, учитывающую член H_2 (так называемое взаимодействие спин-орбита).

ГК-5.11.

Показать, что квадрупольный момент атома водорода равен

$$Q_0 = -\frac{j-\frac{1}{2}}{j+1}\overline{r^2}\left\{\overline{r^2} = \frac{n^2}{2}\left(5n^2+1-3l(l+1)\left(\frac{\hbar^2}{\mu e^2}\right)^2\right\}.\right.$$

ГК-5.12.

Определить суммарную вероятность возбуждения и ионизации атома трития H^3 при β-распаде. Вычислить также вероятности возбуждения n-го уровня.

ГК-5.13.

Найти энергию основного состояния двухэлектронной системы в поле ядра с зарядом Z вариационным методом. В качестве допустимых волновых функций взять произведение водородных функций с эффективным зарядом Z'. Релятивистскими поправками пренебречь.

ГК-5.14.

Волновую функцию атома гелия с достаточной степенью приближения можно положить равной следующему выражению:

$$\psi = \frac{Z'^3}{\pi a^3}e^{-\frac{Z'(r_1+r_2)}{a}}\left(Z' = \frac{27}{16}\right) \text{ (см. задачу 13§7}\Big).$$

Показать, что электростатический потенциал, создаваемый атомом, равен

$$\varphi(r) = 2e\left(\frac{1}{r}+\frac{Z'}{a}\right)e^{-\frac{2Z'r}{a}}.$$

ГК-5.15.

Воспользовавшись приближенной волновой функцией основного состояния атома гелия (см. задачу 13§7), вычислить диамагнитную восприимчивость гелия.

18.1.8 Advanced problems about atoms 2

ГК-5.16.

Определить при помощи вариационного метода энергию основного состояния атома лития с учетом обмена. В качестве собственных волновых функций электронов взять водородные функции для электрона в состоянии $1s$ в виде $\psi_{100} = 2Z_1^{2/2}e^{-Z_1 r}$, для электрона в состоянии $2s$ в виде

$$\psi_{200} = cZ_2^{3/2}e^{-\frac{Z_2 r}{2}}(1-\gamma Z_2 r)$$

Z_1 и Z_2 в этих выражения x являются вариационными параметрами, c определяется из условия нормировки волновой функции ψ_{200}, а γ из условия ортогональности функций ψ_{100}, ψ_{200}. Если бы мы при решении задачи применяли обычную теорию возмущении, то положили бы $Z_1 = Z_2 = 3$. Вводя вариационные параметры Z_1 и Z_2, мы тем самым учитываем экранирующее действие электронов.

ГК-5.17.

Определить смещение энергетических уровней атома вследствие движения ядра. Вычислить величину смещения в атоме гелия для триплетного и синглетного состояний 1 snp, воспользовавшись собственными функциями в форме водородноподобных функций отдельных электронов с эффективным зарядом.

ГК-5.18.

Потенциальная энергия $U(x,y,z)$ является однородной функцией координат с показателем однородности v

$$U(\lambda x, \lambda y, \lambda z) = \lambda^{\nu} U(x,y,z).$$

Доказать, что среднее значение кинетической энергии в состоянии дискретного спектра связано со средним значением потенциальной энергии следующим соотношением $2\bar{T} = \nu\bar{U}$ (теорема вириала).

ГК-5.19. Оценки в рамках модели Томаса-Ферми

Оценить порядок следующих величин согласно модели Томаса-Ферми:
а) среднее расстояние между электроном и ядром; б) средняя энергия кулоновского взаимодействия между двумя электронами в атоме; в) средняя кинетическая энергия электрона; г) энергия, необходимая для полной ионизации атома; д) средняя скорость электронов в атоме; е) средний момент количества движения электрона; ж) среднее радиальное квантовое число электрона.

ГК-5.20.

Выразить приближенно энергию атома через электронную плотность $\rho(\boldsymbol{r})$ согласно модели Томаса-Ферми *).

ГК-5.21.

Показать, что уравнение Томаса-Ферми получается как условие минимума полной энергии при вариации плотности $\rho(\boldsymbol{r})$.
Указание. Воспользоваться результатом предыдущей задачи. При варьировании $E(\rho)$ учесть условие нормировки $\int \rho d\tau = N$ (для нейтрального атома $N = Z$).

ГК-5.22.

Найти вариационным методом наилучшее приближенное выражение для электронной плотности в модели Томаса-Ферми, беря в качестве допустимых функций функции вида $\rho = \frac{Ae^{-x}}{x^3}, x = \sqrt{\frac{r}{\lambda}}$, где A определяется из условия нормировки $\int \rho d\tau = N$ (для нейтрального атома $N = Z$), а λ - параметр, подлежащий варьированию. Определить энергию атома (иона).
Примечание. При выборе вида допустимых функций учтено то обстоятельство, что точное решение в области малых r имеет особенность вида $\rho \sim \frac{\text{const}}{r^{3/2}}$.

ГК-5.23.

Доказать справедливость теоремы вириала для модели Томаса-Ферми.

ГК-5.24.

На основании теоремы вириала доказать, что в модели Томаса-Ферми в нейтральном атоме энергия электростатического взаимодействия электронов составляет $\frac{1}{7}$ от величины взаимодействия электронов с ядром.

ГК-5.25.

Вычислить энергию полной ионизации атома (иона) в приближени,и Томаса-Ферми.

ГК-5.26.

Определить смещение энергетических уровней атома, возникающее вследствие конечности размеров ядра. Потенциал внутри ядра ($r < a$) считать постоянным (физически это означает, что электрический заряд ядра распределен по поверхности сферы радиуса a).

ГК-5.27.

Рассчитать значение $\psi^2(0)$ для валентного s-электрона в атоме с большим Z, используя квазиклассическое приближение.

ГК-5.28.

Определить слагаемое напряженности магнитного поля в центре атома водорода, создаваемое орбитальным движением электрона. Вычислить эту величину для состояния $2p$.

ГК-5.29.

Как изменится выражение для магнитного момента атома водорода в случае учета движения ядра?

ГК-5.30.

Определить расстояние между термами сверхтонкой структуры для s-электрона атома водорода.

ГК-5.31.

Определить энергию сверхтонкой структуры одноэлектронного атома, орбитальный момент количества движения которого не равен нулю.

ГК-5.32. Поле в диамагнитном атоме

Диамагнитный атом находится во внешнем магнитном поле. Определить величину напряженности индуцированного магнитного поля в центре атома.

Solution

В диамагнитных атомах равен нулю не только полный момент, но равны нулю порознь как результирующий орбитальный момент, так и результирующий спиновый момент электронов. Вследствие прецессии электрон приобретает добавочную скорость

$$v' = \frac{e}{2\mu c}[\boldsymbol{\mathcal{H}}, \boldsymbol{r}].$$

Обозначая через A векторный потенциал внешнего магнитного поля $A = \frac{1}{2}[\boldsymbol{\mathcal{H}}, \boldsymbol{r}]$, последнее соотношение можно переписать в виде

$$v' = \frac{e}{\mu c}A.$$

Плотность тока, возникающего вследствие прецессий электронных оболочек, равна

$$J = \frac{e}{\mu C}A\rho(r),$$

где $p(r)$ - плотность заряда в точке r (заряд электрона равен - e). Определим сперва векторный потенциал A' индуцированного магнитного поля

$$A'(r) = \frac{e}{2\mu c^2}\int [\boldsymbol{\mathcal{H}}, \boldsymbol{r}]\frac{\rho\,(r')}{|r - r'|}d\tau'.$$

$$\frac{1}{r_{12}} = \frac{1}{\sqrt{R^2 + r^2 - 2Rr\{\cos\theta\cos\theta + \sin\theta\sin\theta\cos(\Phi - \varphi)}} = \sum_{i,m}\sqrt{\frac{4\pi}{2l+1}}\frac{Y^*_{lm}(\theta,\Phi)Y_{lm}(\vartheta,\varphi)}{Y_{l0}(0)}\begin{cases}\frac{r^l}{R^{l+1}}, & r < R,\\ \frac{R^l}{r^{l+1}}, & r > R,\end{cases}$$

$$A'(r) = \frac{e}{6\mu c^2}[\boldsymbol{\mathcal{H}}, \boldsymbol{r}]\cdot\left\{\frac{1}{r^3}\int\limits_{r'<r} r^2 p\,(r')\,d\tau' + \int\limits_{r>r}\frac{p\,(r')}{r'}d\tau'\right\}.$$

С помощью последнего выражения легко вычислить напряженность магнитного поля в направлении оси z.

Напряженность равна

$$e^{\mathcal{H}'}{}_z = \left(\frac{e_G\ell}{2\mu c^2 r^5}\right)\left(z^2 - \frac{1}{3}r^2\right)_{r'<r}\int^{r^2} p\,(r')\,d\tau' + \frac{e\mathscr{E}}{3\mu c^2}\int\limits_{r'>r}\frac{p\,(r')}{r'}d\tau'.$$

Индуцированное поле в центре атома, т. е. поле, действующее на ядро

$$\mathscr{C}'_z(0) = \frac{e\mathscr{C}}{3\mu c^2}\int\frac{p\,(r')}{r'}d\tau' = \frac{e\mathscr{C}}{3\mu c^2}\,\vartheta\,(0),$$

зависит от электростатического потенциала $\varphi(0)$, производимого электронами.

В модели Томаса-Ферми

$$\varphi(0) = -1,588\frac{Ze}{b}, \quad \text{где} \quad b = 0,858\frac{a}{Z^{1/3}}, \quad a = \frac{h^2}{\mu e^2},$$

и, следовательно,

$$\mathscr{H}'_z(0) = -0,319\cdot 10^{-4}Z^{4/3}\mathscr{H}\mathscr{H}$$

ГК-5.33.

Решить предыдущую задачу в случае гелия.

ГК-5.34.

Указать возможные значения полного момента у состояний ${}^1S, {}^3S, {}^3P, {}^2D, {}^4D$.

18.1.9 Advanced problems about atoms 3

ГК-5.35.

Какие состояния (термы) могут осуществляться для двух электронов а) $nsn's$, б) $nsn'p$, в) $nsn'd$, г) $npn'p$. §71

ГК-5.36. Термы по конфигурации (!!!!!!)

Указать возможные термы следующих конфигурации: а) $(np)^3$, б) $(nd)^2$, в) $ns\,(n'p)^4$,

ГК-5.37. Термы по элементам (!!!)

Определить основные термы следующих элементов: O, Cl, Fe, Co, As, La.

Указание. Для определения необходимо воспользоваться эмпирическими установленными правилами.

1. Наименьшей энергией обладает терм с наибольшим значением S при данной конфигурации электронов и наибольшим (возможным при этом S) значением L (правило Хунда).

2. Для нормального состояния атома $J = |L - S|$, если в не вполне заполненной оболочке находится не более половины максимально возможного для нее числа электронов и $J = L + S$, если оболочка заполнена более чем наполовину.

ГК-5.38.

Определить четность основных термов элементов K, Zn, B, C, N, O, Cl.

39.

Система из N электронов характеризуется N тройками квантовых чисел n, l, m_l. Определить число состоянии, соответствующих данному значению M_S проекции суммарного спина.

40.

Найти число состояний, связанных с конфигурацией nl^x.

41.

Показать, что если $x \leqslant 2l + 1$, то терм с наибольшим значением L для конфигурации nl^x будет синглетным с $L = xl - \frac{1}{4}x(x-2)$, если x четно, или дублетным с $L = xl - \frac{1}{4}(x-1)^2$, если x нечетно.

42.

Из волновых функций одноэлектронной проблемы построить собственные функции, характеризуемые квантовыми числами S, L, M_S, M_L для конфигурации p^3.

Указание. Рассмотреть действие операторов $\left(\hat{L}_x - i\hat{L}_y\right)$ и $\left(\hat{S}_x - i\hat{S}_y\right)$ на антисимметричные функции нулевого приближения.

43.

Получить собственные функции для каждого из двух термов ${}^2D$ конфигурации d^3.

44.

Два электрона движутся в центрально-симметричном поле. Электростатическое взаимодействие электронов будем считать возмущением. Найти энергию возмущения первого порядка для термов конфигурации $npn'p$.

Указание. Сумма корней векового уравнения равна сумме диагональных элементов, входящих в это уравнение.

45.

Показать, что спин-орбитальное возмущение, определяемое формулой $\hat{V}_{SL} = A\hat{\mathbf{S}}\hat{\mathbf{L}}$, обладает тем свойством, что среднее возмущение всех состояний терма (терм характеризуется числами L и S) равно нулю.

46.

Найти расщепление уровней атома в случае слабого магнитного поля, когда $\frac{e\hbar}{2\mu c}\mathscr{H} \ll |\Delta E_{JJ'}|$, где $\Delta E_{JJ'}$ - расстояние между уровнями в мультиплете.

47.

Найти пределы изменения множителя Ланде g при заданных значениях L и S.

48.

Показать, что для термов ${}^4D_{1,2}, {}^5F_1, {}^6G_{3/2}$ отсутствует линейное по полю расщепление.

49.

Определить множитель Ланде для одноэлектронного атома (водород, щелочные металлы) непосредственно при помощи собственных функций Паули (см. задачу 20§4).

50.

Выразить магнитный момент атома через множитель Ланде.

51.

Определить расщепление терма одноэлектронного атома в случае среднего поля $\frac{eh}{2\mu c}\mathscr{E} \sim |\Delta E_{jj}|$.

Решения

1

Из написанного неравенства получаем:

$$\int |\nabla\psi|^2 d\tau + Z\int \left(\nabla|\psi|^2\nabla r\right) d\tau + Z^2\int (\nabla r)^2|\psi|^2 d\tau \geqslant 0$$

Производя во втором члене интегрирование по частям и замечая, что $(\nabla r)^2 = 1$, а $\Delta r = \frac{2}{r}$, имеем:

$$\frac{1}{2}\int |\nabla\psi|^2 d\tau - \int \frac{Z}{r}|\psi|^2 d\tau \geqslant -\frac{Z^2}{2}\int |\psi|^2 d\tau.$$

Левая часть неравенства препставляет среднее значение оператора Гамильтона $*)\hat{H} = -\frac{1}{2}\Delta - \frac{Z}{r}$ в состоянии Ч. Нижнее значэние энергии $-\frac{Z^2}{2}$ достигается в состоянии с волновой функцией (????), удовлетворяющей уравнению первого порядка

$$\nabla\psi_0 + Z\psi_0\nabla r = 0,$$

откуда следует, что

$$\Psi_0 \sim e^{-Zr}$$

5

Вычисляем сначала волновые функции в импульсном представлении по общей формуле

$$\varphi(\boldsymbol{p}) = \frac{1}{(2\pi\hbar)^{3/3}} \iiint e^{-i\frac{pr}{\hbar}} \psi(\boldsymbol{r}) d\tau.$$

Для состояния $1s$ находим:

$$\varphi_{1s}(p) = \frac{1}{\pi} \left(\frac{2a}{\hbar}\right)^{s_i:} \frac{1}{\left(\frac{p^2a^2}{\hbar^2}+1\right)^2}.$$

Аналогично этому для состояния $2s$ получаем:

$$\varphi_{2s}(p) = -\frac{1}{2\pi} \left(\frac{2a}{\hbar}\right)^{s/2} \frac{\frac{p^2a^2}{\hbar^2}-\frac{1}{4}}{\left(\frac{p^2a^2}{\hbar^2}+\frac{1}{4}\right)^3}.$$

Состоянию $2p$ соответствуют 3 собственных функции ($m_2 = -1, 0, +1$)

$$\varphi_{2p}^{(0)}(p) = -i\frac{1}{\pi} \left(\frac{a}{\hbar}\right)^{3/2} \frac{p_z a}{\hbar\left(\frac{p^2a^2}{\hbar^2}+\frac{1}{4}\right)^3},$$

$$\varphi_{2p}^{(\pm1)}(p) = -\frac{i}{\sqrt{2}\pi} \left(\frac{a}{\hbar}\right)^{3/2} \frac{(p_x \pm ip_y)\, a}{\hbar\left(\frac{p^2a^2}{\hbar^2}+\frac{1}{4}\right)^3}.$$

С помощью этих выражений находим распределсние по импульсам (нормированное):

$$\mathfrak{w}(p) = |\varphi(p)|^2.$$

1+5

$\sqrt{r^2 - r^2} = \frac{\sqrt{n^2(n^2+2)-l^2(l+1)^2}}{2}$.
$\to$ В единицах $e = h = \mu = 1$. При заданном n минимальное значение это выражение имеет для «круговых орбит», т. е. при $l = n-1$

$$\sqrt{\overline{r^2} - \overline{r^2}} = \frac{1}{2} n\sqrt{2n+1}, \quad \frac{\sqrt{\overline{r^2} - \bar{r}^2}}{\bar{r}} = \frac{1}{\sqrt{2n+1}}.$$

1+6

При $n_1 = 1, n_2 = 0, m = 0$

$$\psi_{1,0,0}(\xi, \eta, \varphi) = -\frac{1}{\sqrt{2}} R_{20}(r) Y_{00}(i, \varphi) +$$
$$+ + \frac{1}{\sqrt{2}} R_{21}(r) Y_{10}(i, \varphi).$$

1+8

В неквантовой релятивистской механике функция Гамильтона имеет вид

$$H = \sqrt{\mu^2c^4 + p^2c^2} - \mu c^2 + U(r) \approx \frac{p^2}{2\mu} + U(r) + H_1,$$

причем

$$H_1 = -\frac{p^4}{8\mu \cdot c^3}.$$

Будем теперь сиитать p оператором $p = -i\hbar\nabla$, а H_1 рассмотрим как малое возмущение. Тогда в исходном приближении имэем уравнение Шредингера $\left[\frac{\hat{p}^2}{2\mu} + U(r)\right] \circlearrowleft = E\psi$, а искомая поправка к энергии в состоянии n, l, m

$$\Delta E_1 = -\frac{1}{8\mu^3 c^2}\int \psi^* \hat{p}^4 \psi d\tau = -\frac{1}{2\mu c^2}\int \psi^* (E - U(r))^2 \psi d\tau =$$
$$= \frac{3E^2}{2\mu c^2} - \frac{\left(\frac{\mu e^4}{\hbar^2}\right)^2}{n^3 \mu c^2 (2l+1)} = \left[\frac{2}{8n^4} - \frac{1}{(2l+1)n^3}\right]\frac{\mu e^4}{\hbar^2}\left(\frac{e^2}{\hbar c}\right)^2.$$

1+9

Вместо того чтобы исходить из невозмущенных волновых функций определенными l_z и s_z и затем решать секулярное уравнение, удобно выбрать в качестве исходных волновых функций собственные функции с определенным $\boldsymbol{l}^2$ и j^2, где $\hat{\boldsymbol{j}} = \hat{\boldsymbol{l}} + \hat{\boldsymbol{s}}$ — полный момент, коммутирующий, как нетрудно проверить, с H_2. Замечая, что по классу рассматриваемых функций справедливы соотношения

$$\hat{\boldsymbol{j}}^2 = j(j+1) = l(l+1) + s(s+1) + 2\hat{\boldsymbol{l}},$$

находим:

$$\Delta E_2 = \vec{H}_2 = \frac{j(j+1) - l(l+1) - s(s+1)}{4\mu^2 c^2}\hbar^2 \overline{\left(\frac{1}{r}\frac{d\bar{C}}{dr}\right)}$$

Для атома водорода $U = -\frac{e^2}{r}$ и поскольку

$$\frac{\overline{1}}{r^3} = \frac{1}{n^3 (l+1)\left(l+\frac{1}{2}\right) l}\left(\frac{\mu e^2}{\hbar^2}\right)^3,$$

находим окончательно:

$$\Delta E_2 = \frac{\mu e^4}{\hbar^2}\left(\frac{e^2}{\hbar c}\right)^2 \frac{j(j+1) - l(l+1) - s(s+1)}{4n^3 l\left(l+\frac{1}{2}\right)(l+1)}.$$

Эту формулу можно записать короче, так как в нашем случае $s = 1/2$ и возможны два случая $j = l - 1/2$ и $j = l + 1/2$. Как легко проверить, при этом

$$2\hat{\boldsymbol{l}}\hat{\boldsymbol{s}} = j(j+1) - l(l+1) - s(s+1) = \begin{cases} l & \text{при } j = l + \frac{1}{2} \\ -(l+1) & \text{при } j = l - \frac{1}{2}, \end{cases}$$

так что для любых j и l

$$\Delta E_2 = \frac{\mu e^4}{\hbar^2}\left(\frac{e^2}{\hbar c}\right)^2 \frac{1}{2n^3}\left(-\frac{1}{j+\frac{1}{2}} + \frac{1}{l+\frac{1}{2}}\right).$$

Складывая ΔE_2 с пооправкой, учитывающей зависимость массы от скорости ΔE_1 (см. предыдущую задачу), получаем:

$$\Delta E = \frac{\mu e^4}{\hbar^2}\left(\frac{e^2}{\hbar c}\right)\frac{1}{n^3}\left(\frac{3}{8n} - \frac{1}{2j+1}\right).$$

Это выражение не зависит от l, т. е. два уровня с одинаковым j и разными l имеют одинаковую 9 иергию (вырождены).

1+11

При β-распаде япро тритня превращается в ядро изотопа гелия He^3. Влияние β-распада на атомный электрон заключается по существу в том, что за жороткое время $t \ll \frac{j^3}{\mu e^4}$ потенциальная энергия электрона в атоме изменяется и вместо $U = -\frac{e^2}{r}$ становится равной $U = -\frac{2e^2}{r}$. Время t можно оценить как время пролета β-электрона через атом

$$t \sim \frac{a_0}{v},$$

где $a_0 = \frac{\hbar^2}{\mu c^2}$, $\approx$ - скорость β-электрона. Поскольку энергия β-электрона порядка нескольких *кэв*, находим $t \sim 0{,}1\frac{\hbar^3}{\mu e^4}$. Волновая функция электрона не успевает измениться за время t, что следует из уравнения Шредингера:

$$\delta\psi \sim \frac{e^2}{r}\frac{t}{i\hbar}\psi \ll \psi.$$

Разложим волновую функцию электрона по собственным функциям электрона в поле $Z = 2$.

$$\psi = \sum_n c_n\psi_n + \int c_{k_k}\psi_{i_i}d\boldsymbol{k}$$

Козффициенты разложения

$$c_n = \int \psi_n d\tau,$$
$$c_{\boldsymbol{E}} = \int \psi_n \bigcup_{\boldsymbol{s}} d\tau$$

определяют вероятность возбуждения

$$w_n = \sum |c_n|^2$$

и ионизации

$$\mathfrak{W}_{\text{НОН}} = \int |c_{\boldsymbol{l_k}}|^2 d\boldsymbol{k}.$$

Поскольку $\longleftarrow$ - сферически-симметрична, то c_n и c_k отличны от нуля лишь в том случае, когда состояния n, k являются s-состояниями ($l = 0$).

Поскольку

находим:

$$R_{n0}^{(Z)} = 2\left(\frac{Z}{n}\right)^{3/2} e^{-\frac{Z\cdot}{n}} F\left(-n+1, 2, \frac{2Zr}{n}\right),$$

$$c_n = \int_0^\infty R_{n0}^{(Z)} R_{10}^{(Z')} r^2 dr =$$

$$= \frac{8}{\left(Z' + \frac{Z}{n}\right)^3}\left(\frac{ZZ'}{n}\right)^{3/2} F\left(\cdots n+1, 3, 2, \frac{2Z}{nZ'+Z}\right).$$

Полагая $Z = 2, Z' = 1$, получаем для $n = 1$:

$$c_1 = \frac{16\sqrt{2}}{27},$$

т. е. вероятность того, что ион He^3 будет в основном состоянии $w_1 = |c_1|^2 = \left(\frac{8}{9}\right)^3 = 0,70$. Следовательно, суммарная вероятность возбуждения и ионизации будет равна $1 - w_1 = 0,30$. Для $n = 2, c_2 = -\frac{1}{2}, w_2 = 0,25$.

С помощью формулы

$$F(\alpha, \beta, \gamma, x) = (1-x)^{\gamma-\alpha-\beta} F(\gamma-\alpha, \gamma-\beta, \gamma, x)$$

находим:

$$w_n = |c_n|^2 = \frac{2^9 n^5 (n-2)^{2n-4}}{(n+2)^{2n+4}}$$

Приведем значения вероятностей возбуждения, вычисленных с помощью этой формулы, цля нескольких первых уровней:

$$w_1 = \left(\frac{8}{9}\right)^3, \quad w_2 = \frac{1}{4}, \quad w_3 = \frac{2^9 3^j}{5^{10}} = 1,3^{\%}/$$
$$w_4 = \frac{2^{23}}{2^{12}3^{12}} \approx 0,39^{0}\%$$

1+12

Гамильтониан имеет следующий вид (все расчеты будем производить в атомных единицах $e = \hbar = \mu = 1$)

$$\hat{H} = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}.$$

Согласно вариационному принципу надо вычислить интеграл

$$E(Z') = \int \psi^*(r_1, r_2)\, \hat{H}'_{\top}(r_1, r_2)\, d\tau_1 d\tau_2$$

и определить величину Z' из условия $\frac{dE}{dZ'} = 0$.
B нашем случае

$$\psi(r_1, r_2) = ce^{-Z'(r_1 + i_2)},$$

причем нормировочная постоянная $c = \frac{Z'^3}{\pi}$.
Интегралы от первых четырех членов легко вычисляются

$$\int \psi(r_1, r_2) \left\{ -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \frac{Z}{r_1} - \frac{Z}{r_2} \right\} \times$$
$$\times \psi(r_1, r_2)\, d\tau_1 d\tau_2 = Z'^2 - 2ZZ'.$$

Что касается интеграла с $\frac{1}{r_{12}}$, то его удобно вычислить в эллиптических координатах:

$$s = r_1 + r_2, \quad t = r_1 - r_2, \quad u = r_{12},$$
$$d\tau_1 d\tau_2 = \pi^2 \left(s^2 - t^2\right) u ds dt du,$$
$$-u \leqslant t \leqslant u, \quad 0 \leqslant u \leqslant s \leqslant \infty.$$

В результате вычисления имеем:

$$\int \psi^2(r_1, r_2) \frac{1}{r_{12}} d\tau_1 d\tau_2 =$$
$$= \pi^2 c^2 \int_0^{\infty} ds \int_0^{s} du \int_{-u}^{+r} dt e^{-2Z's} \frac{s^2 - t^2}{u} u = \frac{5}{8} Z'.$$

Окончательно получаем:

$$E(Z') = Z'^2 - 2ZZ' + \frac{5}{8} Z'.$$

Из условия минимума $E(Z')$ находим:

$$Z' = Z - \frac{5}{16}.$$

При этом значении Z' энергия основного состояния

$$E = -\left(Z - \frac{5}{16}\right)^2.$$

Чтобы получить представление о точности проведенного расчета, вычислим ионизационный потенциал гелия ($Z = 2$) и сравним результат с экспериментальными данными. Ионизационный потенциал гелия $I_{\text{не}}$ равняется разности энергий однократно ионизированного атома гелия и нейтрального атома гелия в основном состоянии. Значение $I_{\text{не}}$ равно

$$I_{\text{He}} = 0,84 : 6 \text{ ат. ел.} \ = 1,695 Ry *).$$

Экспериментальное значение $I_{\text{He}} = 1,810$.
*) 1 ат. ед. энергии $= 2Ry = 27$ эв. Экспериментально известны также ионизационные потенциалы других двухэлектронных систем $\text{Li}^+, \text{Be}^{++}$и т. д. Сравнивая их с вычисленными, получим:

Элемент	He ($Z = 2$)	Li^+ ($Z = 3$)	Be^{++} ($Z = 4$)	B^{+++} ($Z = 5$)	C^{++++} ($Z = 6$)
Вычисление $I(Ry)$ . . .	1,6952	5,445	11,195	18,945	28,695
Экспериментальное $I(Ry)$	1,810	5,560	11,307	19,061	28,816

Результаты вычисления энергии основного состояния находятся в удовлетворительном согласии с опытом.

1+14

У атома гелия в нормальном состоянии орбитальный и спиновый моменты равны нулю. Вследствие этого гелий обладает диамагнитными свойствами. Диамагнитная восприимчивость, рассчитанная на один грамм-атом, дается следующим выражением:

$$\chi = -\frac{e^2 N_A}{6\mu c^2}\left(\overline{r_1^2} + \overline{r_2^2}\right),$$

где

$$\overline{r_1^2} + \overline{r_2^2} = \int \left(r_1^2 + r_2^2\right)\psi^2 d\tau_1 d\tau_2$$

N_A–число Авогадро. Приближенное выражение для волновой функции основного состояния атома гелия

$$\circlearrowleft (r_1, r_2) = \frac{Z'^3}{\pi a^3} e^{-Z'(r_1+r_2)!a}.$$

Вычисление среднего значения $\overline{r_1^2} + \overline{r_2^2}$ с помощью этой функции приводит к следующему результату:

$$\overline{r_1^2} + \overline{r_2^2} = \frac{2a^2}{Z'^2}.$$

Подставляя это значение в выражение для диамагнитной восприимчивости, находим:

$$\chi = -1,67 \cdot 10^{-6}.$$

Экспериментальное значение диамагнитной восприимчивости

$$x = (1,90 \pm 0,02) \cdot 10^{-6}.$$

1+15

Введем для удобства следующие обозначения:

$$Z_1 = \alpha, \quad Z_2 = 2\beta, \quad 2Z_1^{8/2} = a, \quad cZ_2^{3/2} = b$$

Из условий ортогональности и нормировки находим:

$$\gamma Z_2 = \frac{1}{2}(\alpha + \beta), \quad b^2 = \frac{12\beta^5}{\alpha^2 - \alpha\beta + \beta^2}.$$

В новых обозначениях 1 и ψ_2 будут иметь вид
$\psi_1 = \psi_{100} = ae^{-\alpha r}Y_{00}, \quad \psi_2 = \psi_{200} = b\left[1 - \frac{1}{3}(\alpha + \beta)r\right]e^{-\beta r}Y_{00}$
Приближенная волновая функция атома лития, находящегося в основном состоянии, может быть представлена следующим образом:

$$\Phi = \frac{1}{\sqrt{3!}}\left|\begin{array}{ccc} \psi_1(1)\eta_+(\sigma_1) & \psi_1(2)\eta_+(\sigma_2) & \psi_1(3)\eta_+(\sigma_3) \\ \psi_1(1)\eta_-(\sigma_1) & \psi_1(2)\eta_-(\sigma_2) & \psi_1(3)\eta_-(\sigma_3) \\ \psi_2(1)\eta_+(\sigma_1) & \psi_2(2)\eta_+(\sigma_2) & \psi_2(3)\eta_+(\sigma_3) \end{array}\right|,$$

где $\eta_+\left(\frac{1}{2}\right) = 1, \eta_+\left(-\frac{1}{2}\right) = 0, \eta_-\left(\frac{1}{2}\right) = 0, \eta_-\left(-\frac{1}{2}\right) = 1$. В этом состоянии $S = 1/2, M = 1/2$.
Оператор Гамильтона *) в данном случае имеет вид

$$\hat{H} = \sum_{i=1}^{3}\left\{-\frac{1}{2}\Delta_i - \frac{Z}{r_i}\right\} + \frac{1}{r_{12}} + \frac{1}{r_{23}} + \frac{1}{r_{31}}.$$

Проведем вычисление энергии в состоянии Ф.
Кинетическая энергия электрона в состоянии $1s$ равна

$$T_1 = \int\left\{-\psi_1\frac{1}{2}\Delta\psi_1\right\}d\tau = \int_0^\infty\left(\frac{d\psi_1}{dr}\right)^2 r^2 dr = \frac{1}{2}\alpha^2.$$

*) В атомных единицах $e = \hbar = \mu = 1$. В состоянии $2s$

$$T_2 = \frac{\beta^2}{6} + \frac{\beta^4}{a^2 - \alpha\beta + \beta^2}.$$

Энергия взаимодействия внутреннего электрона с ядром

$$U_1 = -\int \frac{Z\psi_1^2}{r} d\tau = Za^2 \int_0^\infty \frac{e^{-2rr}}{r} r^2 dr = -Z\alpha$$

внешнего электрона с ядром

$$U_2 = -\frac{Z\beta}{2} + \frac{Z\beta^2}{2} \frac{\alpha - 2\beta}{\alpha^2 - \alpha\beta + \beta^2} \text{ (в случае лития } Z = 3)$$

Энергия кулоновского взаимодействия внутренних электронов

$$K_{11} = \iint \frac{1}{r_{12}} |\psi_1(r_1)|^2 |\psi_1(r_2)|^2 d\tau_1 d\tau_2 = \frac{5}{8} a.$$

Энергия взаимодействия внутренних электронов с внешним

$$2K_{12} = 2 \iint \frac{1}{r_{12}} |\psi_1(r_1)|^2 |\psi_2(r_2)|^2 d\tau_1 d\tau_2 =$$
$$= = 2\alpha - \frac{2\alpha^3}{(\alpha+\beta)^2} - \frac{\alpha^4\beta(3\alpha+\beta)}{(\alpha+\beta)^3(\alpha^2-\alpha\beta+\beta^2)}.$$

Энергия обменного взаимодействия двух электронов с параллельными спинами

$$A = 2a^2b^2 \int_0^\infty e^{-(\alpha+\beta)r_2} \left[1 - \frac{1}{3}(\alpha+\beta)r_2\right] r_2^2 dr_2 \times$$
$$\times \int_{r_2}^\infty e^{-(\alpha+\beta)r_1} \left[1 - \frac{1}{3}(\alpha+\beta)r_1\right] r_1 dr_1 =$$
$$= \frac{4\alpha^3\beta^5}{(\alpha+\beta)^5(\alpha^2-\alpha\beta+\beta^2)}.$$

Полагая $\beta = \lambda.\alpha$, получаем:

$$2T_1 + T_2 = T = \alpha^2\varphi_1(\lambda)$$
$$2U_1 + U_2 + K_{11} + 2K_{12} - A = -\alpha\varphi_2(\lambda)$$
$$E = \alpha^2\varphi_1(\lambda) - \alpha\varphi_2(\lambda)$$

Минимум энергии осуществляется при значениях α и λ, удовлетворяющих условиям

$$\frac{\partial E}{\partial \alpha} = 0, \quad \frac{\partial E}{\partial \lambda} = 0$$

Илй

$$2\alpha\varphi_1(\lambda) - \varphi_2(\lambda) = 0, \quad \alpha\varphi_1'(\lambda) - \varphi_2'(\lambda) = 0.$$

Исключая α, получаем:

$$\frac{\varphi_1'(\lambda)}{\varphi_1(\lambda)} - \frac{2\varphi_2'(\lambda)}{\varphi_2(\lambda)} = 0, \quad \lambda = 0,2846.$$

Соответствующие значения α и β равны

$$\alpha = 2,694, \quad \beta = 0,767.$$

Подставляя найденные значения вариационных параметров в E, получаем для энергии нормального состояния атома лития значение

$$E = -7,414 \text{ ат. ед. или } E = -200,8 \text{ эв.}$$

Экспериментальное значение $E = -202,54$ эв. Применяя теорию возмущений, т. е. полагая $\alpha = 3, \beta = 3/2$, мы получим для энергии основного состояния менее точное, чем при вариационном методе, значение $E = -7,05$ или в электрон-вольтах

$$E = -190,84gB.$$

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Рассмотрим оператор кинетической энергии ядра $\hat{T}$. В системе центра инерции

$$P + \sum p_i = 0,$$

где $\boldsymbol{P}$ - импульс ядра, p_i - импульсы электронов, $\hat{T}$ имеет вид

$$\hat{T} = \frac{\hat{P}^3}{2M} = \frac{\left(\sum \hat{p}_i\right)^2}{2M} = \sum \frac{\hat{p}_i^2}{2M} + \sum_{i>k} \frac{\hat{p}_i \hat{p}_k}{M}.$$

Поскольку отношение массы электрона к массе ядра $\frac{m}{M} \ll 1$ - искомое смещение, можно вычислить по теории возм уцений

$$\Delta E = \int u^* \hat{T} \psi d\tau$$

причем ψ - волновая функция электронов в поле бесконечно тяжелого неподвижного ядра.

Первый член в выражении для $\hat{T}$ отличается лишь множителем $\frac{m}{M}$ от кинетической энергии электронов, которая по теореме вириала равна энергии атома с обратным знаком. Таким образом, ΔE представляется в виде суммы двух членов

$$\Delta E = \Delta E_1 + \Delta E_2,$$

$$\Delta E_1 = -\frac{m}{M} E, \quad \Delta E_2 = \frac{1}{M} \int \psi^* \sum_{i>k}^{\top} \hat{\boldsymbol{p}}_i \hat{p}_k \psi d\tau.$$

Рассмотрим более подробно ΔE_2. Если в качестве у(??) взять произведение волновых функций отдельных электронов, то член ΔE_2 обратился бы в нуль, так как средний импульс электрона в связанном состоянии всегда равен нулю. Однако, если должным образом симметризовать такую волновую функцию, ΔE_2 будет отлично от нуля. Симметризованную собственную функцию атома гелия запишем в виде

$$\psi'(r_1, r_2) = \frac{1}{\sqrt{2}} \left[\psi_1(r_1)\psi_2(r_2) \pm \psi_1(r_2)\psi_2(r_1)\right],$$

причем верхний знак относитсяк парагелию (полный спин $S = 0$), а нижний к ортогелию ($S = 1$).

Представляя это выражение в формулу для ΔE_2, получаем:

$$\Delta E_2 = \pm \frac{1}{M} \left| \int \psi_1^* \hat{p}_1^{\omega_2} d\tau \right|^2.$$

Матричный элемент импульса отличен от нуля, лишь когда $\Delta l = 0, \pm 1$ и, таким образом, ΔE_2 обращается в нуль для состояний 1 snd, 1 snf и т. д.

Беря для $1s$-электрона и для np-электрона водородные функции с эффективным зарядом соответственно Z_1 и Z_2

$$\psi_{1s}(r) = \sqrt{\frac{Z_1^3}{\pi}} e^{-Z_1 r},$$

$$\psi_{np} = Y_{10} \frac{2Z_2^2}{3} \frac{\sqrt{n^2-1}}{n^2} r e^{-\frac{Z_{2^*}}{n}} F\left(-n+2, 4; \frac{2Z_2 r}{n}\right),$$

получим:

$$\Delta E_2 = \pm \frac{m}{M} \frac{64}{3} (Z_1 Z_2)^5 \frac{(Z_1 n - Z_2)^{2n-4}}{(Z_1 n + Z_2)^{2n+4}} n^3 \left(n^2 - 1\right)$$

причем верхний знак относится к паратерму $1\,\mathrm{snp}\,{}^1P$, нижний - К ортотерму $1\,\mathrm{sip}\,{}^3P$.

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Пусть $\psi(x, y, z)$ является решением уравнения Шредингера, относящимся к дискретному спектру энергии. Рассмотрим однопараметрическое семейство нормированных функций вида $\lambda^{3/2}\psi(\lambda x, \lambda y, \lambda z)$.

Выражение

$$I(\lambda) = \lambda^3 \int \left\{ \frac{\hbar^2}{2\mu} |\nabla \psi(\lambda x, \lambda, y, \lambda z)|^2 + \right.$$

$$\left. + U(x, y, z) |\psi(\lambda x, \lambda y, \lambda z)|^2 \right\} dxdydz,$$

как функция λ, должно иметь экстремум при $\lambda = 1$, т. е.

$$\left(\frac{dI}{d\lambda}\right)_{\lambda=1} = 0.$$

Переходя к новым переменным интегрирования $\lambda x, \lambda y, \lambda z$, получаем:

$$I(\lambda) = \lambda^2 \bar{T} + \lambda^{-v} \bar{U}.$$

Откуда находим:

$$2\bar{T} - \nu \bar{U} = 0.$$

Теорема вириала легко обобщается на случай системы многих частиц.

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а) $Z^{-1/2} \frac{\hbar^2}{\mu \cdot e^2}$,
б) $Z^{1/s} \frac{\mu e^4}{\hbar^2}$,
в) $Z^{4/\mu} \frac{\mu e^4}{\hbar^2}$,
г) $Z^{7/3} \frac{\mu e^4}{\hbar^2}$,
л) $Z^{2/\frac{e^2}{\hbar}}$,
е) $Z^{1/s}\hbar$
ж) $Z^{1/}$.

20

Полная энергия складывается из трех частей: кинетической энергии электронов T, энергии взаимодействия электронов с ядром U_{ne} и энергии взаимодействия электронов между собой U_{ee}. Два последних слагаемых имеют следующий вид:

$$U_{ne} = -\int \frac{Z}{r} \rho d\tau,$$
$$U_{ee} = \frac{1}{2} \int \frac{\rho(\boldsymbol{r}) \rho(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} d\tau d\tau'.$$

Чтобы вычислить кинетическую энергию, рассмотрим бесконечно-малый элемент объема атома $d\tau$. Число электронов с импульсами, лежащими в пределах $\boldsymbol{p}$ и $\boldsymbol{p} + dp$, пропорционально фазовому объему и равняется

$$dn = \frac{8\pi p^2 dp d\tau}{(2\pi)^3} = \frac{p^2 dp d\tau}{\pi^2}.$$

Плотность электронов получится интегрированием по от 0 до некоторого максимального $p = p_0$.

$$\rho = \frac{p_0^3}{3\pi^2}.$$

Кинетическая энергия электронов в объеме $d\tau$

$$dT = \int_0^{p_0} \frac{p^2}{2} dn = \frac{p_0^5}{10\pi^2} d\tau.$$

Выразив в этой формуле p_0 через и интегрируя по объему атома, находим кинетическую энергию электронов

$$T = \frac{1}{10\pi^2} \left(3\pi^2\right)^{5/3} \int \rho^{5/3} d\tau.$$

Окончательно для полной энергии получаем:

$$E = T + U_{ne} + U_{ee} =$$
$$= \frac{\left(3\pi^2\right)^{5/s}}{10\pi^2} \int \rho^{5/3} d\tau - Z \int_e^2 \frac{\rho}{r} d\tau + \frac{1}{2} \iint \frac{\rho(r) \rho(r')}{|r - r'|} d\tau d\tau'.$$

22

Элемент объема, выраженный через x, имеет вид

$$d\tau = 4\pi r^2 dr = 8\pi\lambda^3 x^5 dx.$$

Вычисляем кинетическую энергию

$$T = \frac{12\left(3\pi^2\right)^{5/3}}{25\pi}\lambda^3 A^{5/3}$$

и энергию взаимодействия электронов с ядром

$$U_{ne} = -8\pi A\lambda^2 Z.$$

Для того чтобы вычислить $U_{ee} = \frac{1}{2}\iint \frac{p(\boldsymbol{r})p(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}d\tau d\tau'$, найдем сначала потенциал, создаваемый электронами φ_e. Решая уравнение Пуассона

$$\Delta\varphi_e = 4\pi\rho_s$$

получим:

$$\varphi_e = -\frac{16\pi A\lambda^2}{x^2}\left[1 - e^{-x}(x+1)\right]$$

Вычисляя теперь U_{ee} с помощью теоремы Грина, находим:

$$U_{ee} = -\frac{1}{2}\int \varphi_e \rho d\tau = 16\pi^2 A^2\lambda^5.$$

Из условия нормировки определяем A

$$\int \rho d\tau = 16\pi A\lambda^3 = N$$

Подставляя $A = \frac{N}{16\pi\lambda^3}$ в выражения для T, U_{ne}, U_e, получим:

$$T = \frac{12}{25\pi}\left(\frac{3\pi N}{16}\right)^{8/3}\frac{1}{\lambda^2},$$
$$U_{ne} = -\frac{ZN}{2\lambda},$$
$$U_{ee} = \frac{N^2}{16\lambda}.$$

Минимум $E = T + U_{ne} + U_{ee}$ достигается при

$$\lambda = \frac{9}{25}\left(\frac{3\pi N}{16}\right)^{2/3}\frac{1}{Z - \frac{N}{8}}$$

и составляет

$$E = \frac{25}{36}\left(\frac{16}{3\pi}\right)^{2/3} N^{1/3}\left(Z - \frac{N}{8}\right)^2 \text{ ат. ед.}$$

Для нейтрального атома

$$E = \frac{25\cdot 49}{36\cdot 64}\left(\frac{16}{3\pi}\right)^{3/3} Z^{7/3} = 0,758Z^{7/3} \text{ ат. ед.}$$

1+22

Пусть $\rho(\boldsymbol{r})$ - выражение для электронной плотности в модели Томаса-ферми. Тогда $\rho(r)$ осуществляет минимум энергии атома

$$E = \frac{\left(3\pi^2\right)^{5/3}}{10\pi^2} \int^{5/3} d\tau - Z \int \frac{p}{r} d\tau + \frac{1}{2} \iint \frac{p(\boldsymbol{r}) p\left(\boldsymbol{r}'\right)}{|\boldsymbol{r} - \boldsymbol{r}'|} d\tau d\tau'.$$

Если в это выражение вместо p подставить функцию $\lambda^3 p(\lambda r)$, удовлетворяющую тому же условию нормировки, что и $\rho(\boldsymbol{r})$, то получим $E(\lambda) = \lambda^2 T + \lambda U$, где T - кинетическая, а U - потенциальная энергия электронов в атоме. Поскольку E ((.) должно иметь минимум при $\lambda = 1$, находим, что должно выполняться равенство

$$2T + U = 0$$

выражающее теорему вириала.

1+23

Энергия взаимодействия между электронами может быть записана в виде

$$U_{ee} = -\frac{1}{2} \int \varphi_e p d\tau = \frac{Z}{2} \int \frac{p}{r} d\tau - \frac{1}{2} \int \varphi p d\tau,$$

где φ_e - потенциал, создаваемый электронами, а φ - потенциал самосогласованного поля, включающий поле ядра

$$\varphi = \varphi_e + \frac{Z}{r}.$$

В модели Томаса-Ферми выполняются соотношения

$$\frac{p_0^2}{2} = \varphi - \varphi_0, \quad \rho = \frac{p_0^3}{3\pi^2},$$

где p_0 - максимальный импульс, φ_0 - потенциал на границе атома. Исключая отсюда p_0 и выражая в формуле (1) φ через р, находим:

$$U_{ee} = \frac{Z}{2} \int \frac{p}{r} d\tau - \frac{\left(3\pi^2\right)^{2/3}}{4} \int p^{5/3} d\tau - \frac{\varphi_0 N}{2}.$$

Первые два члена лишь множителями отличаются от энергии взаимодействия электронов с ядром

$$U_{ne} = -Z \int \frac{p}{r} d\tau$$

и кинетической энергии

$$T = \frac{3\left(3\pi^2\right)^{2/3}}{10} \int p^{5/3} d\tau.$$

Таким образом,

$$U_{ee} = -\frac{1}{2} U_{ne} - \frac{5}{6} T - \frac{\varphi_0 N}{2}.$$

Подставляя сюда значения T из теоремы вириала

$$2T = -U_{ne} - U_{ee}$$

окончательно находим:

$$U_{ee} = -\frac{1}{7} U_{ne} - \frac{6}{7} \varphi_0 N.$$

Для нейтрального атома $(N = Z)\varphi_0 = 0$ и

$$U_{ee} = -\frac{1}{7} U_{ne}.$$

1+24

Энергия полной ионизации равна полной энергии электронов, взятой с обратным знаком. Используя теорему вириала, находим (см. предыдущую задачу):

$$E_{\text{пог}} = -\frac{3}{7}U_{ne} + \frac{3}{7}\varphi_0 N.$$

Преобразуем выражение

$$U_{ne} = -Z\int \frac{p}{r}d\tau$$

следующим образом: введем потенциал φ_e, создаваемый электронами

$$\Delta\varphi_e = 4\pi p$$

и используем теорему Грина

$$U_{ne} = -\frac{Z}{4\pi}\int \frac{\Delta\varphi_e}{r}d\tau = Z\varphi_e(0)$$

(поверхностный интеграл на границе атома равен нулю и $\Delta\frac{1}{r} = -4\pi\delta(r)$).
Итак,

$$E_{\text{ион}} = -\frac{3}{7}Z\varphi_e(0) + \frac{3}{7}N\varphi_0.$$

Переходя к томас-фермиевским единицам

$$r = xbZ^{-1/3}, \quad b = \frac{1}{2}\left(\frac{3\pi}{4}\right)^{2/3}, \varphi - \varphi_0 = \frac{Z^{4/3}}{b}\frac{\chi(x)}{x},$$

находим:

$$\varphi_e(r) = \varphi - \frac{Z}{r} = \varphi_0 - \frac{Z^{4/3}}{b}[1-\chi(x)],$$

и поскольку для малых x

$$\chi(x) = 1 - ax + \frac{4}{3}x^{3/2},$$

где $a = a_0 = 1,58$ для нейтрального атома (для положительного иона $a > a_0$), то окончательно

$$E_{\text{нон}} = \frac{3}{7}\frac{Z^{7/3}}{b}a - \frac{3}{7}\frac{(Z-N)^2 Z^{1/3}}{bx_0},$$

x_0 - радиус $(Z-N)$ - кратного иона.

1+25

Потенциал точечного кулоновского центра совпадает с потенциалом заряженной по поверхности сферы вне этой сферы, поскольку полный заряд в обоих случаях одинаков. Внутри сферы разница двух потенциалов составляет

$$\Delta\varphi = -Ze\left(\frac{1}{r} - \frac{1}{a}\right).$$

Изменение потенциальной энергии электронов атома

$$\Delta U = -Ze^2\sum_{i=1}^{N}\left(\frac{1}{r_i} - \frac{1}{a}\right)\varepsilon(r_i),$$

где введена вспомогательная функция

$$\varepsilon(r) = \begin{cases} 1 & r < a \\ 0 & r > a \end{cases}$$

Смещение уровней энергии в первом приближении теории возмущений

$$\Delta E = -Ze^2\int |\psi|^2 \sum_{i=1}^{N}\left(\frac{1}{r_i} - \frac{1}{a}\right)\varepsilon(r_i)\, d\tau_1 ... d\tau_N.$$

Нтегрирование по всем переменным, кроме одной, дает:

$$\int |\Psi\left(r_1 ... r_N\right)|^2 d\tau_2 ... d\tau_N = \frac{1}{N} p(r)$$

где $p(r)$ - элект ронная плотность.
Таким образом,

$$\Delta E = -Ze^2 \int \rho(r) \left(\frac{1}{r} - \frac{1}{a}\right) \varepsilon(r) d\tau.$$

Воспользуемся тем, что $p(r)$ мало изменяется в области $r < a$. Вынося эту величину за знак интеграла в точке $r = 0$, получаем

$$\Delta E = -Ze^2 p(0) \frac{2\pi}{3} a^2.$$

\section{7. Волновая функция s-электрона

$$\psi_n(r) = \frac{1}{\sqrt{4\pi}} \frac{\chi_n(r)}{r},$$

где χ_n удовлетворяет уравнению

$$\gamma_n'' + \frac{2\mu}{\hbar^2} \left[E_n - U(r)\right] \chi_n = 0$$

и нормировочному условию

$$\int_0^\infty \chi_n^2 dr = 1.$$

Решение уравнения для χ_n в квазиклассическом приближении имеет вид

$$\chi n = \frac{A_n}{\sqrt{p_n}} \cos\left(\frac{1}{\hbar} \int_0^r p_n dr + \varphi\right),$$

где

$$p_n = \sqrt{2\mu \left[E_n - U(r)\right]}.$$

Это решение, однако, непригодно в области малых r. В самом деле, если r мало $\left(r \ll \frac{\hbar^2}{Z^{1/3} \mu e^2}\right)$ то, во-первых, можно пренебречь экранированием поля ядра и положить $U(r) = -\frac{Ze^2}{r}$; во-вторых, можно также пренебречь E_n по сравнению с $U(r)$. Подставляя $p = \sqrt{\frac{2\mu Ze^2}{r}}$ в условие применимости квазиклассическ ого приближения

$$\frac{d\left(\frac{h}{p}\right)}{dr} \ll 1,$$

получаем:

$$Z \gg \frac{h^2}{Z\mu e^2}.$$

Чтобы получить для $/n$ выражение, пригодное в области малых r, вернемся к исходному уравнению и заменим в нем $U(r)$ на $-\frac{Ze^2}{r}$, а также пренебрежем E_n:

$$\gamma_n'' + \frac{2\mu}{n^2} \frac{Ze^2}{r} \gamma_n = 0.$$

Это уравнение имеет решение

$$y_n = C_n \sqrt{r} J_1\left(2\sqrt{\frac{2\mu Ze^2 r}{\hbar^2}}\right).$$

Чтобы найти связь между постоянными C_n и A_n, замечаем, что область применимости квазиклассического решения (1)

$$r \gg \frac{\hbar^2}{Z\mu e^2}$$

и область применимости решения (2), в которой пренебрегается экранированием поля ядра,

$$r \ll \frac{h^2}{Z^{1/s}\mu e^2}$$

при больших Z перекрываются и поэтому решения (1) и (2) в области $\frac{\hbar^2}{Z\mu e^2} \ll r \ll \frac{\hbar^2}{Z^{1/3}\mu e^2}$ должны совпадать.

Покажем, что вид решений (1) и (2) одинаков в общей области применимости. Для этого положим в (1) $p = \sqrt{\frac{2\mu Ze^2}{r}}$. Тогда получаем

$\chi_n = \frac{A_n \sqrt[4]{\cdot \bar{r}}}{\sqrt[4]{2\mu Ze^2}} \cos\left(\frac{2\sqrt{2\mu \cdot Ze^2 r}}{h} + \varphi\right) \frac{\hbar^2}{Z\mu e^2} \ll r \ll \frac{h^2}{Z^{1/3}\mu e^2}$.

Условие $r \gg \frac{\hbar^2}{Z\mu e^2}$ означает, что аргумент бесселевой функции в (2) велик. Но для больших аргументов ($x \gg 1$)

$$J_1(x) \approx \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{3\pi}{4}\right).$$

Таким образом, решение (2) принимает виль

$$\chi_n = C_n \sqrt{r} \sqrt{\frac{h}{\pi\sqrt{2\mu Ze^{2r}}}} \cos\left(\frac{2\sqrt{2\mu Ze^{3r}}}{h^2} - \frac{3\pi}{4}\right)$$
$$\frac{h^2}{Z\mu e^2} \ll r \ll \frac{h^2}{Z^{1/s\mu e^2}}.$$

Сравнивая эту формулу с (3), найдем:

$$\varphi = -\frac{3\pi}{4}, \quad A_n = C_n\sqrt{\frac{\hbar}{\pi}}.$$

Теперь можно найти $\psi^2(0)$ При $x \ll 1$ имеем $J_1(x) = \frac{x}{2}$ и с помощью формулы находим:

$$\left.\frac{\gamma_n}{r}\right|_{r\to 0} = C_n\sqrt{\frac{2\mu \cdot Ze^2}{\hbar^2}} = \sqrt{\frac{2\pi\mu \cdot Ze^2}{\hbar^3}} A_n.$$

Следовательно,

$$\psi_n^2(0) = \frac{\mu Z c^2}{2h^3} A_n^2.$$

Постоянную A_n определим из условия нормировки

$$\int_0^\infty \gamma_n^2 dr = A_n^2 \int_0^\infty \frac{\cos^2\left(\frac{1}{\hbar}\int_0^r p_n dr - \frac{3\pi}{4}\right)}{\sqrt{2\mu[E_n - U(r)]}} dr \approx$$
$$\approx \frac{A_n^2}{2} \int_0 \frac{dr}{\sqrt{2\mu[E_n - U(r)]}} \quad 1.$$

Дифференцируя по n условие квантования,

$$\int \sqrt{2\mu\left[E_n - U(r)\right]} dr = \pi(n+\gamma)\hbar,$$

которое определяет E_n как функцию от n, находим:

$$\mu \frac{dE_n}{dn} \int \frac{dr}{\sqrt{2\mu\left[E_n - U(r)\right]}} = \pi\hbar.$$

Сравнивая последнее выражение с условием нормировки, получим:

$$A_n^2 = \frac{2\mu}{\pi h} \frac{dE_n}{dn}$$

и окончательно

$$\psi_n^2(0) = \frac{Ze^2\omega^2}{\pi\hbar^4} \frac{dE_n}{dn}.$$

Для неэкранированного кулоновского поля $E_n = -\frac{Z^2}{2n^2}\frac{\mu e^4}{\hbar^2}$ и найденное из формулы (4) $\iota_n^2(0) = \frac{Z^3}{\pi n^3}\left(\frac{\mu e^2}{\hbar^2}\right)^3$ совпадает с полученным из точного расчета. *B* атомной спектроскопии для уровней энергии возбужденных состояний валентного электрона часто используется формула

$$E_n = -\frac{\mu\rho^4}{2!^2}\frac{1}{(n-\sigma)^3},$$

где о-так называемая поправка Ридберга, слабо зависящая от n. Приняв для E_n эту формулу, получаем:

$$\psi^2(0) = \frac{Z}{\pi}\frac{\mu^3 e^6}{\hbar^6}\frac{\left(1-\frac{d\sigma}{dn}\right)}{(n-\sigma)^3}.$$

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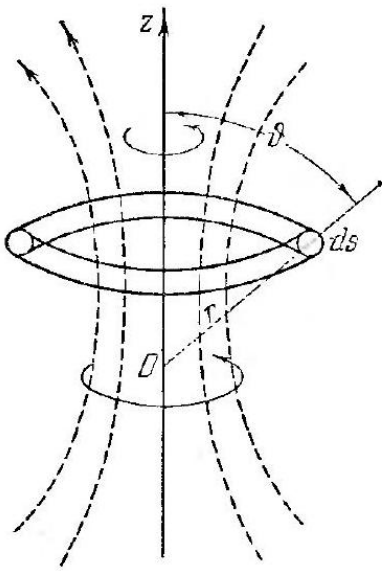
Пусть электрон находится в стационарном состоянии, с определенным значением проекции момента импульса m. Волновая функция такого состояния равна

$$\psi_{nlm}(r,8,\varphi) = R_{nl}(r)P_l^{(m)}(\cos\vartheta)e^{im\varphi}.$$

Плотность электрического тока в состоянии (???) в полярной системе координат $r,\{,\varphi$ имеет вид

$$J_r = J_8 = 0, \quad J_\varphi = -\frac{|e|\hbar m}{\mu r\sin\vartheta}|\psi_{nlm}|^2.$$

Очевидно, что вектор напряженности магнитного поля будет направлен по оси Z.



Рй. 28.

Круговой ток силы dJсо– здает в точке O (см. рис. 28) магнитное поле, напряженность которого равна

$$d\%_z = \frac{dJ}{rc}2\pi\sin^2\vartheta; \quad \text{так как} \quad dJ = J_\varphi r d\vartheta dr$$

ТО

$Q_z = \frac{2\pi|e|hm}{\mu c}\int\limits_0^\infty \frac{R^2}{r}dr\int\limits_0^\pi |P_\eta^{(m)}|^2\sin\vartheta d\vartheta = -\frac{m|e|\hbar}{\mu\cdot c}\int\limits_0^\infty \frac{R^2}{r}dr.$

Этот результат можно получить и иным способом.

Как известно из электродинамики, напряженность магнитного поля, создаваемого при движении заряда, равна (запаздывание не учитывается)

$$\mathscr{H} = \frac{e}{\mu c}\frac{1}{r^3}[rp] = \frac{e}{\mu c}\frac{1}{r^3}l,$$

где r - радиус-вектор, проведенный из точки наблюдения, l - момент количества движения.

В квантовой теории для определения среднего значения на- пряженности магнитного поля нужно вычислить интеграл вида

$$\overline{\mathscr{A}}_z = -\frac{|e|\hbar}{\mu c}\int \psi^* \frac{\hat{l}_z}{r^3}\psi d\tau; \quad \text{так как} \quad \hat{l}_z\psi = m\psi,$$

ТО

$$\overline{\mathscr{A}\mathscr{H}}_z = -m\frac{|e|\hbar}{\mu c}\frac{\overline{1}}{r^3} = -m\frac{|e|\hbar}{\mu c}\left(\frac{\mu e^2}{\hbar^2}\right)^3 \frac{1}{n^3\left(l+\frac{1}{2}\right)(l+1)}.$$

Среднее значение $\mathscr{H}_x, \mathscr{E}_y$ в нашем случае будет равно нулю вследствие того, что

$$\int \psi^*_{nlm}\hat{l}_y\psi_{nlm}\,d\tau = \int \psi^*_{nlm}\hat{l}_x\psi_{nlm}\,d\tau = 0.$$

Для состояния $2p(m=1)$ получаем:

$$\overline{\mathscr{H}}_z = -\frac{1}{12}\frac{|e|\hbar}{2\mu c}\left(\frac{\mu e^2}{\hbar^2}\right)^3, \quad \text{т. е.} \quad \overline{\mathscr{H}}_z \sim 10^4\ \text{гаусс}.$$

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Магнитный момент частицы равен

$$\mathfrak{M} = \frac{e}{2_1 \cdot c}\int \psi^* \hat{\boldsymbol{l}}\psi d\tau.$$

В случае двух частиц введем новые переменные: координаты центра масс (X, Y, Z) и координаты, характеризующие взаимное расстояние (x, y, z).

Среднее значение магнитного момента, выраженное через новые переменные, будет равно

$$\overline{\mathfrak{M}}_z = \frac{e}{2c}\int \psi^* \left\{\left(\frac{1}{m}+\frac{1}{M}\right)\left(X\frac{\partial}{\partial y} - Y\frac{\partial}{\partial x}\right) + \right.$$
$$\left. + \frac{1}{m+M}\left(x\frac{\partial}{\partial \bar{Y}} - y\frac{\partial}{\partial X}\right) + \frac{m-M}{mM}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\right\}\psi dr,$$

и аналогично для $\bar{\mathfrak{i}}_x$ и $\overline{\mathfrak{M}\mathfrak{i}}_y$.

В стационарном состоянии средние значения координат x, y, z и импульсов $-i\hbar\frac{\partial}{\partial x}, -i\hbar\frac{\partial}{\partial y}, -i\hbar\frac{\partial}{\partial z}$ обращаются в нуль. Вследствие этого последнее выражение упростится и примет вид

$$\overline{\mathfrak{D}}_z = -\frac{e}{2mc}\left(1-\frac{m}{M}\right)\int \psi^* \left\{-i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\right\}\psi d\tau.$$

В этой задаче m - масса электрона, а M - масса ядра.

30.

$\Delta E = 0,00844 \cdot 2,79\frac{Z^3}{n^3}cM^{-1}$.

Для основного состояния водородного атома $(Z = n = 1)$

$$\Delta E = 0,0235\ \text{см}^{-1}.$$

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Для определения энергии необходимо найти напряженность магнитного поля, создаваемого электроном. Вследствие орбитального движения электрона в той точке, в которой находится ядро, возникает магнитное поле, напряженность которого по закону Био и Савара равна

$$\mathfrak{H}_l = \frac{1}{c}\frac{[\boldsymbol{r}j]}{r^3},$$

где r - радиус-вектор, направленный от ядра к электрону, а $\boldsymbol{j} = -e\boldsymbol{z}$ (заряд электрона - e). Введем оператор орбитального момента $\hat{\mathrm{Im}}ath$. Тогда для $\hat{\mathscr{H}}_l$ получим:

$$\hat{\mathscr{H}}_l = -\frac{e\hbar}{\mu c}\frac{1}{r^3}\hat{l}.$$

Вследствие того, что электрон, помимо электрического заряда, имеет спиновый магнитный момент, полная напряженность магнитного поля в указанной точке равна

$$\hat{\mathfrak{H}} = \hat{\mathfrak{H}}_l + \hat{\mathfrak{H}}_s = \frac{e\hbar 1}{\mu \cdot r^3}\left\{\hat{\boldsymbol{s}} - \frac{3(\boldsymbol{r}\hat{s})r}{r^2} - \hat{\boldsymbol{i}}\right\}.$$

Таким образом, оператор энергии сверхтонкой структуры мы можем представить следующим образом:

$$\hat{w} = -\beta\hat{i}\hat{\mathfrak{H}},$$

здесь $\hat{\boldsymbol{i}}$-оператор спина ядра, а $\hat{\hat{i}}$ - магнитный момент. Будем рассматривать $\hat{w}$ как малое возмущение. Невозмущенное состояние характеризуется квантовыми числами $n, j(j = l + 1/2, j = l - 1/2), l$ (предполагаем наличие LS связи). Для определения энергии сверхтонкой структуры мы должны усреднить оператор $\hat{\boldsymbol{w}}$ по состоянию с квантовыми числами

$$f, j, l(\hat{f} = \hat{j} + \hat{i}).$$

На основании формулы
имеем:

$$(\hat{A})^{f_m}_{rm}{}^{r} = \frac{\left(\hat{f}\hat{A}\hat{)}^{f}_{f}\right.}{f(f+1)}(\hat{f})^{f'_m}_{fm}$$

$$(g\hat{\mathcal{Q}})^{nljm'_j}_{nljm_j} = -\frac{e\hbar}{\mu c}\left(\frac{1}{r^3}\right)^{nljm_j}_{nljm_j}\frac{l(l+1)}{j(j+1)}(\hat{j})^{jm'_j}_{jm_j}.$$

Используя это соотношение, легко показать, что оператор $\hat{w}$ может быть представлен в виде

$$\hat{w} = \frac{e\hbar}{\mu, c}\beta\frac{1}{r^3}\frac{l(l+1)}{j(j+1)}(\hat{i}\hat{j}).$$

Отсюда следует, что энергия E сверхтонкой структуры определяется выражением

$$E = \frac{e\hbar}{2\mu c}\beta\left(\overline{\frac{1}{r^3}}\right)\frac{l(l+1)}{j(j+1)}\{f(f+1) - j(j+1) - i(i+1)\}.$$

Таким образом, при учете сверхтонкой структуры каждый терм, характеризуемый числами n, l, j, расщепляется на $2i + 1$ компонент (если $j > i$). Совокупность различных значений f дает правило интервалов для сверхтонкой мультиплетной структуры.

Отметим, что путем простого подсчета числа компонент сверхтонкой структуры в спектре данного изотопа можно определить спин ядра. На рис. 29 изображена сверхтонкая мультиплетная структура D-линий натрия.

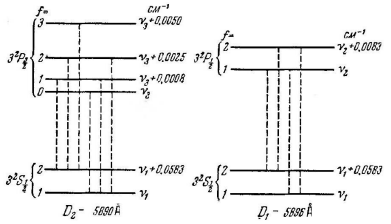

Рис. 29.

Тонкая структура, т. е. наличие дублета (линии $D_1 = 5896$Å, соответствующая переходу $3^2P_{3/2} \to 3^2S_{1/2}$ и $D_2 = 5890$Å, соответствующая переходу $3^2P_{1/2} \to 3^2S_{1/2}$), объясняется спин-орбитальным взаимодействием (см. задачу 10§7).

1+32

$\mathscr{H}_z'(0) = -\frac{27}{24}\frac{e^2\mathscr{G}C}{\mu c^2 a} = -0,599 \cdot 10^{-4}\mathscr{H}$.
${}^1S_0, {}^3S_1, {}^3P_{0,1,2}, {}^2D^3_{3/2}, 5/2, {}^4D_{1,2}, 3/2, 5/z, 7/2$
а) ${}^1S_0{}^3S_1$
б) $1P_1 8P_{012}$
в) ${}^1D^3_2 D_{123}$
г) ${}^1S_0{}^3S^1_1P_1, {}^3P_{012}{}^1D^3_2D_{123}$.

1+35

а) ${}^4S^2P^2D$
б) ${}^1S^3P^1D^3F^1G$
В) ${}^2S^2P^4P^2D$.

1+36

$\mathrm{O}^3P_2, \mathrm{Cl}^2P_{3/2}, \mathrm{Fe}^2D_4, \mathrm{Co}^4F_{9/2}, \mathrm{As}^4S_{3/2}, \mathrm{La}^2D_{8/2}$.
K, Zn, C, O - четные; B, N, Cl - нечетные. 39. Если все тройки квантовых чисел различны, то число состояний равно числу сочетаний из N по $\frac{N}{2} + M_s$, т. е.

$$g\left(M_s\right) = \mathrm{C}_N^{\frac{1}{2}N + M_s}.$$

Если имеется N' пар одинаковых троек квантовых чисел n, l, m_l, то

$$g\left(M_s\right) = \mathrm{C}_{N-2N'}^{\frac{1}{2}\left(N-2N'\right)+M_s}.$$

1+39

Число состояний равно

$$\frac{N_L\left(N_l-1\right)\ldots\left(N_l-x+1\right)}{x!}, \text{ где } N_l = 2(2l+1).$$

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С целью краткости антисимметричную волновую функцию вида

$$\Phi = \frac{1}{N!}\begin{vmatrix} \psi_{n^1 l^1 m_l^1 m_s^1}(\xi_1) & \psi_{n^1 l^1 m_l^1 m_s^1}(\xi_2) & \cdots & \psi_{n^1 l^1 m_l^1 m_s^1}(\xi_N) \\ \psi_{n^2 l^2 m_l^2 m_s^2}(\xi_1) & \psi_{n^2 l^2 m_l^2 m_s^2}(\xi_2) & \cdots & \psi_{n^2 l^2 m_l^2 m_s^2}(\xi_N) \\ \cdots & \cdots & \cdots & \cdots \\ \psi_{n^N l^N m_l^N m_s^N}(\xi_1) & \psi_{n^N l^N m_l^N m_s^N}(\xi_2) & \cdots & \psi_{n^N l^N m_l^N m_s^N}(\xi_N) \end{vmatrix},$$

составленную из функций одноэлектронной проблемы, будем обозначать следующим образом:

$$\Phi\left(n^1 l^1 m_l^1 m_s^1, n^2 l^2 m_l^2 m_s^2, \ldots, n^N l^N m_l^N m_s^N\right).$$

Рассмотрим действие симметричного онератора

$$\left(\hat{L}_x - i\hat{L}_y\right) = \sum_{i=1}^{N}\left(\hat{l}_x^i - i\hat{l}_y^i\right)$$

na антисимметричную функцию

$$\Phi\left(n^1 l^1 m_l^1 m_s^1, n^2 l^2 m_l^2 m_s^2, \ldots, n^N l^N m_l^N m_s^N\right)$$

Легко видеть, что
$\left(\hat{L}_x - i\hat{L}_y\right)\Phi\left(n^1 l^1 m_l^1 m_s^1, n^2 l^2 m_l^2 m_\varepsilon^2, \ldots\right) =$
$= \sqrt{\left(l^1 + m_l^1\right)\left(l^1 - m_l^1 + 1\right)}\Phi\left(n^1 l^1 m_l^1 - 1m_s', n^2 l^2 m_l^2 m_s^2, \ldots\right) +$
$+\sqrt{\left(l^2 + m_l^2\right)\left(l^2 - m_l^2 + 1\right)}\Phi\left(n^1 l^1 m_l^1 m_s^1, n^2 l^2 m_l^2 - 1m_s^2, \ldots\right) + \ldots$
$\ldots + \sqrt{\left(l^N + m_l^N\right)\left(l^N - m_l^N + 1\right)}\Phi\left(n^1 l^1 m_l^1 m_8^1, \ldots, n^N l^N m_l^N - 1m_j^N\right)$

Результаты действия оператора $\hat{S}_x - i\hat{S}_y$ аналогичны, только вместо m_l понижаются на 1 значения m_s.

Если волновая функция является собственной функцией четырех коммутирующих операторов $\hat{S}^2, \hat{L}^2, \hat{S}_z, \hat{L}_z$, то действие операторов $\left(\hat{L}_x - i\hat{L}_y\right)$ и $\left(\hat{S}_x - i\hat{S}_y\right)$ сводится к следующему:

$$\left(\hat{L}_x - i\hat{L}_y\right)\Phi\left(SLM_SM_L\right) =$$
$$= \sqrt{\left(L + M_L\right)\left(L - M_L + 1\right)}\Phi\left(SLM_SM_L - 1\right),$$
$$\left(\hat{S}_x - i\hat{S}_y\right)\Phi\left(SLM_SM_L\right) =$$
$$= \sqrt{\left(S + M_S\right)\left(S - M_S + 1\right)}\Phi\left(SLM_S - 1M_L\right).\Big)$$

После этих предварительных замечаний приступим непосредственно к решению нашей задачи.

В рассматриваемом случае мы имеем дело с эквивалентными электронами, поэтому квантовые числа nl можно везде опустить. Значение проекции спинового момента будем иногда указывать посредством индексов (????), расположенных над m_l.

Приведем для конфигурации p^3 классификацию состояний по M_S и M_L (ограничиваемся только неотрицательными значениями) и получающиеся в каждом случае термы

$$\begin{array}{l} M_SM_L \\ \frac{3}{2}0\Phi\left(1^+, -1^+, \quad 0^+\right) \quad \left[{}^4S\right] \quad \Phi_1 \\ \left.\begin{array}{llll} \frac{1}{2} & 0 & \Phi\left(1^+, -1^+, \quad 0^-\right) & \\ & & \Phi\left(1^-, -1^+, \quad 0^+\right) & {}^4S \\ & & {}^2P & \\ & & \left(1^+, -1^-, \quad 0^+\right) & \Phi_2 \\ {}^2D & & & \end{array}\right] \begin{array}{l} \Phi_3 \\ \Phi_4 \end{array} \\ \frac{1}{2}2\Phi\left(1^i, 1^-, \quad 0^+\right) \quad \left[{}^2D\right] \quad \Phi_7 \end{array}$$

Затем вычислим действие операторов $\left(\hat{L}_x - i\hat{L}_y\right), \left(\hat{S}_x - i\hat{S}_y\right)$ на некоторые из приведенных выше состояниЙ

$$\left(\dot{L}_x - i\hat{L}_y\right)\Phi_{\tilde{\mathrm{D}}} = \sqrt{2}\left(\Phi_3 - \Phi_2\right)$$
$$\left(\hat{L}_x - i\hat{L}_y\right)\Phi_6 = \sqrt{2}\left(\Phi_2 - \Phi_4\right),$$

$$\begin{array}{llll} \frac{1}{2} & 1 & \Phi(1^+, \quad 1^-, -1^+) & \left[\begin{array}{l} {}^2P \\ {}^2D \end{array}\right] \quad \begin{array}{l} \Phi_5 \\ \Phi_6 \end{array} \\ \cdot & & \Phi(1^+, \quad 0^+, \quad 0^-) & \end{array}$$

$$\left(\hat{L}_x - i\hat{L}_y\right)\Phi_7 = \sqrt{2}\left(\Phi_5 - \Phi_6\right),$$
$$\left(\hat{S}_x - i\hat{S}_y\right)\Phi_1 = \Phi_2 + \Phi_3 + \Phi_4,$$

Φ_1 есть волновая функция состояния ${}^4S$ с $M_S = \frac{3}{2}, M_L = 0$.

Действуя на эту функцию оператором $\left(\hat{S}_x - i\hat{S}_y\right)$, согласно (1) получим:

$$\left(\hat{S}_x - i\hat{S}_y\right)\Phi\left({}^4S, \frac{3}{2}, 0\right) = \sqrt{3}\Phi\left({}^4S, \frac{1}{2}, 0\right),$$

так как

$$\left(\hat{S}_x - i\hat{S}_y\right)\Phi_1 = \Phi_2 + \Phi_3 + \Phi_4,$$

ТО

$$\Phi\left({}^4S, \frac{1}{2}, 0\right) = \frac{1}{\sqrt{3}}\left(\Phi_2 + \Phi_3 + \Phi_4\right)$$

Аналогично для терма ${}^2D$ получим следующие волновые функции:

$$\Phi\left({}^2D,\frac{1}{2},2\right)=\Phi_7,$$
$$\Phi\left({}^2D,\frac{1}{2},1\right)=\frac{1}{\sqrt{2}}\left(\Phi_5-\Phi_6\right),$$
$$\Phi\left({}^2D,\frac{1}{2},0\right)=\frac{1}{\sqrt{6}}\left(\Phi_3-2\Phi_2+\Phi_4\right).$$

Состояние ${}^2P,\frac{1}{2},1\left(M_S=\frac{1}{2},M_L=1\right)$ представляет собой линейную комбинацию состояний Φ_5 и Φ_6, ортогональную к состоянию ${}^2D,\frac{1}{2},1$. Из этих соображений находим:

$$\Phi\left({}^2P,\frac{1}{2},1\right)=\frac{1}{\sqrt{2}}\left(\Phi_5+\Phi_6\right),$$

и далее

$$\Phi\left({}^2P,\frac{1}{2},0\right)=\frac{1}{\sqrt{2}}\left(\Phi_3-\Phi_4\right).$$

Таким же самым способом можно получить волновые функции, соответствующие отрицательным значениям проекции.

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Как следует из приведенной ниже таблицы для определения собственных функций двух термов ${}^2D$, необходимо вычислить сперва собственные функции термов ${}^2H,{}^2G,{}^4F,{}^2F$.

M_SM_L

$\frac{1}{2}5\Phi\left(2^+,2^-,1^+\right)\quad\Phi_1\quad\left[{}^2H\right]$

$$\begin{array}{cccccc}
 & \frac{1}{2} & 3 & \Phi\left(2^+,2^-, & 1^+\right) & \Phi_4 \quad {}^2H \\
\Phi\left(2^+,1^+,\right. & & 0^-\right) & & \Phi_5 \quad {}^2G & \\
 & \Phi\left(2^+,1^-,\right. & & 0^+\right) & \Phi_6 \quad {}^4F & \\
\Phi\left(2^-,1^+,\right. & & 0^+\right) & & \Phi_7 \quad 2^2F &
\end{array}$$

$$\begin{array}{cccccc}
 & \frac{1}{2}2 & \Phi\left(2^+,2^-, & -2^+\right) & \Phi_8 & {}^2H \\
\Phi\left(2^+,1^+,\right. & -1^-\right) & & \Phi_9 & {}^2G & \\
 & & \Phi\left(2^+,1^-, & -1^+\right) & \Phi_{10} & {}^4F \\
 & & \Phi\left(2^-,1^+, & -1^+\right) & \Phi_{11} & {}^2F \\
 & & \Phi\left(2^+,0^+, & 0^-\right) & \Phi_{12} & {}^2D \\
\Phi\left(1^+,1^-,\right. & 0^+\right) & & \Phi_{13} & {}^2D &
\end{array}$$

$\frac{3}{2}3\Phi\left(2^+,1^+,0^+\right)\Phi_{14}$

$\frac{3}{2}2\Phi\left(2^+,1^+,-1^+\right)\Phi_{1\check{a}}$

Найдем сперва результат действия операторов $\left(\hat{L}_x-i\hat{L}_y\right)$, $\left(\hat{S}_x-i\hat{S}_y\right)$ на некоторые из приведенных выше состояний:

$$\left(\hat{L}_x-i\hat{L}_y\right)\Phi_1=-2\Phi_3+\sqrt{6}\Phi_2$$
$$\left(\hat{L}_x-i\hat{L}_y\right)\Phi_2=-2\Phi_z+2\Phi_6+\sqrt{6}\Phi_4$$
$$\left(\hat{L}_x-i\hat{L}_y\right)\Phi_3=-\sqrt{6}^x+\sqrt{6}\Phi_5$$
$$\left(\hat{S}_x-i\hat{S}_y\right)\Phi_{14}=\Phi_i+\Phi_6+\Phi_5$$
$$\left(\hat{L}_x-i\hat{L}_2\right)\Phi_4=-2\Phi_{11}+2\Phi_{10}+2\Phi_6$$
$$\left(\hat{L}_x-i\hat{L}_y\right)\Phi_5=\sqrt{6}\Phi_{12}+\sqrt{6}\Phi_9$$
$$\left(\dot{S}_x-i\hat{S}_y\right)\Phi_{15}=\Phi_{11}+\Phi_{10}+\Phi_8$$
$$\left(\hat{L}_x-i\hat{L}_y\right)\Phi_6=2\Phi_{13}-\sqrt{6}\Phi_{12}+\sqrt{6}\Phi_{10^*}$$
$$\left(\hat{L}_x-i\hat{L}_y\right)\Phi_7=-2\Phi_{13}+\sqrt{6}\Phi_{11}$$

$$\begin{array}{cccccc} \frac{1}{2} & 4 & \Phi(2^+, & 2^-, & 0^+) & \Phi_2 \\ & & \Phi(2^+, & 1^+, & 1^-) & \Phi_3 \end{array} \quad \begin{bmatrix} ^2H \\ ^2G \end{bmatrix}$$

Волновая функция состояния $^2H, \frac{1}{2}, 5\left(M_S = \frac{1}{2}, M_L = 5\right)$ равна Φ_1, т. е. $\Phi\left(^2H, \frac{1}{2}, 5\right) = \Phi_1$. Применяя оператор $\left(\hat{L}_x - i\hat{L}_y\right)$, получаем:

$$\left(\hat{L}_x - i\hat{L}_y\right)\Phi\left(^2H, \frac{1}{2}, 5\right) = \sqrt{10}\Phi\left(^2H, \frac{1}{2}, 4\right).$$

Так как $\left(\hat{L}_x - i\hat{L}_y\right)\Phi_1 = -2\Phi_3 + \sqrt{6}\Phi_2$, то

$$\Phi\left(^2H, \frac{1}{2}, 4\right) = \frac{1}{\sqrt{10}}\left\{\sqrt{6}\Phi_2 - 2\Phi_3\right\}.$$

Другие, нужные для решения задачи, состояния терма ^2H находим последовательно:

$$\Phi\left(^2H, \frac{1}{2}, 3\right) = \frac{1}{\sqrt{30}}\left\{\sqrt{6}\Phi_4 - 2\Phi_5 + 4\Phi_6 - 2\Phi_3\right\},$$
$$\Phi\left(^2H, \frac{1}{2}, 2\right) = \frac{1}{\sqrt{30}}\left\{\Phi_8 - \Phi_9 + 3\Phi_{10} - 2\Phi_{11} - 3\Phi_{12} + \sqrt{6}\Phi_{13}\right\}.$$

Состояние $\Phi\left(^2G, \frac{1}{2}, 4\right)$ представляет собой линейную комбинацию состояний Φ_2 и Φ_3, ортогональную к состоянию $\Phi\left(^2H, \frac{1}{2}, 4\right)$. Из этих условий определяем волновую функцию $\Phi\left(^2G, \frac{1}{2}, 4\right)$

$$\Phi\left(^2G, \frac{1}{2}, 4\right) = \frac{e^{i\alpha}}{\sqrt{10}}\left\{2\Phi_2 + \sqrt{6}\Phi_3\right\}.$$

Так как состояния разных термов не связаны никакими фазовыми соотношениями, мы можем положить $\alpha = 0$.

Другие состояния терма ^2G получаются посредством последовательного применения оператора $\left(\hat{L}_{sc} - i\hat{L}_y\right)$. Итак, имеем:

$$\Phi\left(^2G, \frac{1}{2}, 4\right) = \frac{1}{\sqrt{10}}\left\{2\Phi_2 + \sqrt{6}\Phi_3\right\},$$
$$\Phi\left(^2G, \frac{1}{2}, 3\right) = \frac{1}{\sqrt{20}}\left\{\sqrt{6}\Phi_4 + 3\Phi_5 - \Phi_6 - 2\Phi_7\right\},$$
$$\Phi\left(^2G, \frac{1}{2}, 2\right) =$$
$$= \sqrt{\frac{3}{140}}\left\{2\Phi_8 + 3\Phi_9 + \Phi_{10} - 4\Phi_{11} + 4\Phi_{12} + \sqrt{\frac{2}{3}}\Phi_{13}\right\}.$$

Для того чтобы решить задачу, нам необходимо еще определить функции $\Phi\left(^4F, \frac{1}{2}, 2\right)$ и $\Phi\left(^2F, \frac{1}{2}, 2\right)$.

Так как $\Phi\left(4F, \frac{3}{2}, 3\right) = \Phi_{14}$, то, действуя оператором $\left(\hat{S}_x - i\hat{S}_y\right)$, получим состояние $\Phi\left(^4F, \frac{1}{2}, 3\right)$:

$\left(\hat{S}_x - i\hat{S}_y\right)\Phi\left(^4F, \frac{3}{2}, 3\right) = \sqrt{3}\Phi\left(^4F, \frac{1}{2}, 3\right) = \left(\hat{S}_x - i\hat{S}_y\right)\Phi_{14}$, $\Phi\left(^4F, \frac{1}{2}, 3\right) = \frac{1}{\sqrt{3}}\left\{\Phi_5 + \Phi_6 + \Phi_7\right\}$

А из состояния $\Phi\left(^4F, \frac{1}{2}, 3\right)$ посредством оператора $\left(\hat{L}_x - i\hat{L}_y\right)$ получаем состояние $\Phi\left(^4F, \frac{1}{2}, 2\right)$:

$$\Phi\left(^4F, \frac{1}{2}, 2\right) = \frac{1}{\sqrt{3}}\left\{\Phi_9 + \Phi_{10} + \Phi_{11}\right\}.$$

Волновая функция $\Phi\left(^2F, \frac{1}{2}, 3\right)$ определится из условия ортогональности ее к трем функциям $\Phi\left(^2H, \frac{1}{2}, 3\right)$, $\Phi\left(^2G, \frac{1}{2}, 3\right), \Phi\left(^4F, \frac{1}{2}, 3\right)$. Нормированная функция $\Phi\left(^2F, \frac{1}{2}, 3\right)$, определенная из этих условий, равна

$$\Phi\left(^2F, \frac{1}{2}, 3\right) = \frac{1}{\sqrt{12}}\left\{-\sqrt{6}\Phi_4 + \Phi_5 + \Phi_6 - 2\Phi_7\right\}.$$

И, наконец,

$$\Phi\left(^2F, \frac{1}{2}, 2\right) = \frac{1}{\sqrt{12}}\left\{-2\Phi_8 + \Phi_9 - \Phi_{10} + \sqrt{6}\Phi_{13}\right\}.$$

Теперь мы имеем четыре состояния с $M_S = \frac{1}{2}$ и $M_L = 2$, $\Phi\left(^2H, \frac{1}{2}, 2\right) =$

$$= \frac{1}{\sqrt{30}} \left\{ \Phi_8 - \Phi_9 + 3\Phi_{10} - 2\Phi_{11} - 3\Phi_{12} + V\overline{6}\Phi_{13} \right\},$$

$\Phi\left({}^2G, \frac{1}{2}, 2\right) =$
$= \sqrt{\frac{3}{140}} \left\{ 2\Phi_8 + 3\Phi_9 + \Phi_{10} - 4\Phi_{11} + 4\Phi_{12} + \sqrt{\frac{2}{3}}\Phi_{13} \right\}$, $\Phi\left({}^4F, \frac{1}{2}, 2\right) = \frac{1}{\sqrt{3}} \{\Phi_9 + \Phi_{10} + \Phi_{11}\}$,
$\Phi\left({}^2F, \frac{1}{2}, 2\right) = \frac{1}{\sqrt{12}} \left\{ -2\Phi_8 + \Phi_9 - \Phi_{10} + \sqrt{6}\Phi_{13} \right\}$.

В эту же группу входят еще два ${}^2D$ состояния. Эти два взаимно ортогональные ${}^2D$ состояния ортогональны также к написанным выше четырем состояниям.

Из условий ортогональности и нормировки получаем следующие ортонормированные функции:

$$\Phi\left(a^2D, \frac{1}{2}, 2\right) = \frac{1}{2} \{-\Phi_8 - \Phi_9 + \Phi_{10} + \Phi_{12}\}$$

$$\Phi\left(b^2D, \frac{1}{2}, 2\right) =$$

$$= \frac{1}{\sqrt{84}} \left\{ -5\Phi_8 + 3\Phi_9 + \Phi_{10} - 4\Phi_{11} - 3\Phi_{12} - 2\sqrt{6\Phi_{13}} \right\}^{\top}$$

Остальные волновые функции ${}^2D$ состояний, соответствующие другим значениям проекции моментов, легко определяются посредством последовательного применения операторов $\left(\hat{L}_x - i\hat{L}_y\right)$ и $\left(\hat{S}_x - i\hat{S}_y\right)$.

44

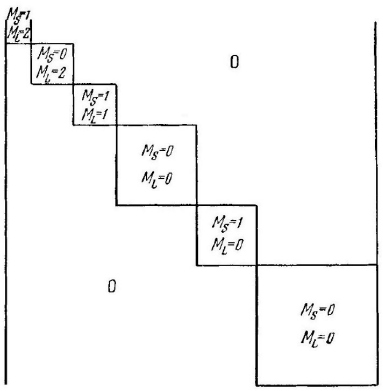
Составим сперва список всех состояний, принадлежащих конфигурации $npn'p$. Ограничимся неотрицательными значениями M_S и M_L

pp		M_S	
		1	0
M_L	2	$\Phi_1(1^+, 1^+)$	$\Phi_2(1^+, 1^-)$ $\Phi_3(1^-, 1^+)$
	1	$\Phi_4(1^+, 0^+)$ $\Phi_5(0^+, 1^+)$	$\Phi_6(1^+, 0^-)$ $\Phi_7(0^+, 1^-)$ $\Phi_8(1^-, 0^+)$ $\Phi_9(0^-, 1^+)$
	0	$\Phi_{10}(1^+, -1^+)\Phi_{11}(0^+, 0^+)$ $\Phi_{12}(-1^+, 1^+)$	$\Phi_{13}(1^+, -1^-)$ $\Phi_{14}(0^+, 0^-)$ $\Phi_{15}(-1^+, 1^-)$ $\Phi_{16}(1^-, -1^+)$ $\Phi_{17}(0^-, 0^+)$ $\Phi_{18}(-1^-, 1^+)$

Из рассмотрения таблицы следует, что данная конфигурация имеет термы ${}^1S, {}^3S, {}^1P, {}^3P, {}^1D$ и ${}^3D$.

При решении задачи в качестве функций нулевого приближения возьмем функции, указанные в таблице.

Так как энергия не зависит от значения проекций M_S и M_L, то матрица возмущения будет представлена в виде субматриц следующим образом:



Обозначим через $\hat{V}$ оператор возмущения. В первой субматрице присутствует только терм ${}^8D$. Следовательно,

$$E^{(1)}\left({}^3D\right) = V_{11}.$$

Во второй субматрице ($M_L = 2, M_S = 0$) комбинируются два терма ${}^3D$ и ${}^1D$,

$$E^{(1)}\left({}^3D\right) + E^{(1)}\left({}^1D\right) = V_{22} + V_{33}.$$

В третьей субматрице ($M_L = 1, M_S = 0$) комбинируются два терма ${}^3D$ и ${}^3P$,

$$E^{(1)}\left({}^3D\right) + E^{(1)}\left({}^3P\right) = V_{44} + V_{65}.$$

В четвертой субматрице ($M_L = 1, M_S = 0$) четыре терма: ${}^3D), {}^1D, {}^3P, {}^1P$

$$E^{(1)}\left({}^3D\right) + E^{(1)}\left({}^1D\right) + E^{(1)}\left({}^3P\right) + E^{(1)}\left({}^1P\right) = V_{66} + V_{77} + V_{88} + V_{99^*}$$

В пятой субматрице ($M_L = 0, M_S = 1$) три терма: ${}^3D, {}^3P, {}^3S$,

$$E^{(1)}\left({}^3D\right) + E^{(1)}\left({}^3P\right) + E^{(1)}\left({}^3S\right) = V_{10,10} + V_{11,11} + V_{12,12}$$

Н, наконец, в шестой ($M_L = 0, M_S = 0$) все термы: ${}^3D, {}^3P$, ${}^3S, {}^1D, {}^1P, {}^1S$

$$\begin{aligned} E^{(1)}\left({}^3D\right) + E^{(1)}\left({}^1D\right) + E^{(1)}\left({}^3P\right) + \\ + E^{(1)}\left({}^1P\right) + E^{(1)}\left({}^3S\right) + E^{(1)}\left({}^1S\right) = \\ = V_{13,13} + V_{14,14} + V_{15,15} + V_{16,16} + V_{17,17} + V_{18,18} \end{aligned}$$

Из этих уравнений легко получить выражение для термов через диагональные матричные элементы:

$$\begin{aligned} E^{(1)}\left({}^3D\right) &= V_{11}, \\ E^{(1)}\left({}^1D\right) &= V_{22} + V_{33} - V_{11}, \\ E^{(1)}\left({}^3P\right) &= V_{44} + V_{55} - V_{11}, \\ E^{(1)}\left({}^1P\right) &= V_{66} + V_{77} + V_{89} + V_{99} + V_{11} - V_{22} - V_{33} - V_{44} - V_{50} \end{aligned}$$

и Т. Д.

1+45

Выражение $\frac{e\hbar}{2\mu c}\left(\hat{L}_z + 2\hat{S}_z\right)$ Эt' является малым возмущением. Рассматриваем рассель-саундеровский тип связи. В этом случае $\hat{H}_0$ коммутирует операторами $\hat{J}^2, \hat{J}_z$, $\hat{\boldsymbol{L}}^2, \hat{\boldsymbol{S}}^2$. Уровни энергии невозмущенного состояния характеризуются квантовыми числами J, L, S. Каждый из этих уровней вырожден по направлению вектора $\hat{\boldsymbol{J}}$, кратность этого вырождения равна $2J + 1$.

Так как недиагональные по $\hat{J}_z$ матричные элементы оператора $\left(\hat{L}_z + 2\hat{S}_z\right)$ равны нулю, то поправка к энергии равна просто среднему значению оператора $\left(\hat{L}_z + 2\hat{S}_z\right)$ в состоянии, характеризуемом квантовыми числами J, JJ_z, L, S. С целью вычисления этого среднего значения положим в формуле (задачи 29§4) $g_1 = 1, g_2 = 2, \hat{J}_1 = \hat{\boldsymbol{L}}, \hat{\boldsymbol{J}}_2 = \hat{\boldsymbol{S}}$. В результате получим:

$$\overline{\hat{L}_z + 2\hat{S}_z} = J_z\left\{\frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}\right\} = J_z g.$$

Согласно сказанному выше искомое расщепление будет равно

$$E^{(1)}_{JLS} = \frac{e\hbar\mathscr{E}}{2\mu c} g J_z.$$

18.1.10 Advanced problems about atoms 4

52.

Найти волновые функции электрона, находящегося в условиях, указанных в предыдущей задаче.

53.

Определить расщепление уровней атома водорода, находящегося в сильном магнитном поле $\left(\frac{e\hbar}{2\mu.c}\mathscr{H} > |E_{nlj} - E_{nlj'}|\right)$. Для применения теории возмущений необходимо потребовать, чтобы энергия атома в магнитном поле была мала по сравнению с разностью энергии различных мультиплетов, т. е.

$$\frac{e\hbar\mathscr{E}}{2\mu c} < |E_{nlj} - E_{n'lj}|.$$

54.

Определить зеемановское расщепление компонент сверхтонкой структуры терма $^2S_{1/2}(j = 1/2, l = 0)$ в случае среднего магнитного поля $\left(\frac{e\hbar}{2\mu c}\mathscr{E} \sim |\Delta E_{ff'}|\right)$. (Расщепление, вызываемое полем одного порядка с интервалами сверхтонкой структуры.)

55.

Показать, что при произвольном значении напряженности магнитного поля сумма изменений энергий, вызванных магнитным полем, по всем состояниям с заданным M_J равна

$$\frac{e\hbar}{2\mu \cdot c}\mathscr{H}M_J \sum \left\{1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}\right\}.$$

Здесь суммирование производится по J, заключенным в пределах $L + S \leqslant J \leqslant |L - S|, J \geqslant M_J$.

56.

Показать, что при помещении атома водорода в однородное электрическое поле а) энергия состояния с квантовыми числами $l = n - 1$, $m = n - 1$ в линейном по полю приближении не изменяется; б) не меняется положение центра тяжести расщепленного терма; в) состояния, отличающиеся только знаком проекции момента, имеют одну и ту же энергию.

57.

Вычислить расшепление уровней атома водорода в слабом электрическом поле (эффект Штарка мал по сравнению с тонкой структурой).

58.

Найти магнитный момент атома водорода, находящегося в слабом электрическом поле.

59

. Вычислить расщепление терма с $n = 2$ атома водорода, находящегося в среднем (по величине напряженности) электрическом поле (эффект Штарка и тонкая структура одного порядка).

60.

Рассмотрим атом, находящийся под действием возмущающего потенциала $\boldsymbol{u}$. Применяя теорию возмущений, получим для волновои функции ψ в первом приближении выражение следующего вида:

$$\psi = \psi_0 + \sum_{n\neq 0} \frac{u_{n0}}{E_0 - E_n}\psi_n,$$

а для энергии

$$E = E_0 + u_{00} + \sum_{n=0} \frac{(u_{n0})^2}{E_0 - E_n}.$$

Для того чтобы в дальнейшем применить вариационный метод, упростим, насколько это возможно, вид ψ. Так как

$$\sum_{n\neq 0}^{\infty} u_{n0}\psi_n = -u_{00}\psi_0 + \sum_{n=0}^{\infty} u_{n0}\psi_n = \psi_0 (u - u_{00}),$$

то ф приближенно запишем следующим образом:

$$\psi \approx \psi_0 \left(1 + \frac{u - u_{00}}{E'}\right)$$

где E' можно в некоторых случаях считать равным среднему значению $E_0 - E_n$. После того, как вид возмущенной волновой функции приближенно установлен, мы можем для определения энергии применить вариационный метод.

Определить вариационным методом энергию атома, находящегося под действием возмущающего потенциала u. Минимум энергии искать в классе допустимых функций вида $\psi = \psi_0(1 + \lambda u)$, где λ-вариационный параметр.

ГК-5.61.

Исходя из результата предыдущей задачи, найти формулу для поляризуемости атома. Определить численные значения коэффициента поляризуемости для атомов водорода и гелия, находящихся в основных состояниях.

ГК-5.62.

Атом водорода находится в параллельных электрическом и магнитном полях. Найти расщепление в случае а) слабых полей (энергия штарковского и зеемановского расщепления меньше энергии тонкой структуры); б) средних полей, для терма с главным квантовым числом $n = 2$.

ГК-5.63.

Атом водорода в состоянии с главным квантовым числом $n = 2$ находится во взаимно перпендикулярных электрическом и магнитном полях. Определить расщепление, предполагая, что поля сильные (энергия электрона во внешнем электрическом и магнитном поле больше энергии тонкой структуры).

Solutions

1+50

Энергия атома в магнитном поле одного порядка со спин-орбитальным взаимодействием. Поэтому оператор спинорбитального взаимодействия, равный $\varphi(r)\hat{i}\hat{s}$ (см. задачу 10 § 7), объединяем с оператором $\frac{e\hbar}{2\mu c}\left(\hat{l_z} + 2\hat{s_z}\right)$ и их сумму

$$V = \varphi(r)\hat{l}\hat{s} + \frac{e\hbar}{2\mu c}\mathscr{H}\left(\hat{l}_z + 2\hat{s}_z\right)$$

рассматриваем как малое возмущение. В невозмущенном состоянии сохраняющимися величинами будут квадрат и проекция орбитального момента, а также квадрат и проекция спина. Нам удобнее взять другой набор сохраняющихся величин. Будем характеризовать стационарное невозмущенное состояние квантовыми числами $n, \boldsymbol{l}, \dot{j}, m_j$ $\left(\hat{l}^2, j^2, \hat{j}_z\right.$ коммутируют с $\left.H_0\right)$. Степень вырождения в случае кулоновского поля равна $2n^2$, в случае центрально-симметричного произвольного поля $2(2l+1)$. Нам нет необходимости решать секулярное уравнение такой высокой степени. Заметим, что в возмущенном состоянии квадрат орбитального момента и проекция полного момента являются интегралами движения. Вследствие этого волновая функция возмущенной задачи должна быть скомбинирована из функций

$$\psi_{nljm_j}{}^{(0)}$$

относящихся к одним и тем же значениям n, l, m_j, т. е. $\psi = c_1\psi^{(0)}\left(n, l, j = l - \frac{1}{2}, m_j\right) + c_2\psi^{(0)}\left(n, l, j = l + \frac{1}{2}, m_j\right)$ или в другой форме

$$+ c_2\frac{R^{(0)}_{nl}}{\sqrt{2l+1}}\begin{pmatrix} \sqrt{l - m_j + \frac{1}{2}}Y_{l,m_j-1/2} \\ -\sqrt{l + m_j + \frac{1}{2}}Y_{l,m_j+1/2} \end{pmatrix}.$$

Матричные элементы оператора $\hat{V}$ равны

$$(\hat{V})^{nlj=l+1_2m}_{nlj=l+1;2m} j = A\frac{l}{2} + e^{\top}\mu_0\mu_0 m_j\left(1 + \frac{1}{2l-1}\right),$$

$$(\hat{V})^{nlj=l-j_{j2}m_j}_{nlj=l-1/2m_j} = -A\frac{l+1}{2} + \mathscr{F}\mu_0 m_j\left(1 - \frac{1}{2l+1}\right),$$

где

$$A = \int_0^\infty R_{nl}(r)\varphi(r)R_{nl}(r)r^2dr, \quad \text{а} \quad \mu_0 = \frac{e\hbar}{2ic}.$$

Значение энергии E находится из решения секулярного уравнения

$$E_{nl}^0 + A\frac{l}{2} + \mathscr{H}\mu_0 m_j\left(1+\frac{1}{2l+1}\right) - E,$$
$$\frac{\partial \mathscr{A}\mu_0}{2l+1}\sqrt{\left(l+\frac{1}{2}\right)^2 - m_j^2}| = 0.$$
$$\frac{\partial l+1}{\left(l+\frac{1}{2}\right)^2 - m_j^2}$$

Обозначим через E_+и E_-энергию одноэлект ронного атома с учетом спин-орбитаиынго взаимодействия, причем E_+ относится к состоянию с $j = l + 1/2$, а E_-с $j = l - 1/2$.

Как следует из решения задачи 10§7,

$$E_+ = E_{nl}^{(0)} + A\frac{l}{2}, \quad E_- = E_{nl}^{(0)} - A\frac{l+1}{2}.$$

$$\Psi = c_1 \frac{R_{nl}^{(0)}}{\sqrt{2l+1}}\begin{pmatrix}\sqrt{l+m_j+\frac{1}{2}}\,Y_{l,\,m_j-1/2}\\ \sqrt{l-m_j+\frac{1}{2}}\,Y_{l,\,m_j+1/2}\end{pmatrix} +$$

$$(\hat{V})_{nlj=l-1/2 m_j}^{nlj=l-1/2 m_j} = (\hat{V})_{nlj=l+1/2 m_j}^{nlj=l+1/2 m_j} = \frac{\mathscr{H}\mu_0}{2l+1}\sqrt{\left(l+\frac{1}{2}\right)^2 - m_j^2}.$$

Решая секулярное уравнение, находим значение E:

$$E = \frac{1}{2}(E_+ + E_-) + e^{\cdot\cdot}\cdot \mu_0 m_j \pm$$
$$\pm\sqrt{\frac{1}{4}(E_+ - E_-)^2 + \mathscr{H}\mu_0\frac{m_j}{2l+1}(E_+ - E_-) + \frac{1}{4}\mathscr{H}^2\mu_{0^2}{}^*}$$

Рассмотрим предельные случаи.

а) В случае слабых полей, т. е. при ${\mu_0}^7 \ll E_+ - E_-$ для энергии получаем следующие выражения:

$$E = E_+ + \mathscr{H}\theta\mu_0 m_j\frac{2l+2}{2l+1},$$
$$E = E_- - \mathscr{E}\theta\mu_0 m_j\frac{2l}{2l+1}.$$

Первое значение энергии соответствует энергии n-го уровня состояния с $j = l + 1/2$, а второе с $j = l - 1/2$ (см. задачу 46 \$7)

б) В случае сильных полей, т. е. при $\mu_0\mathscr{F} \gg E_+ - E_-$ $E = \frac{1}{2}(E_+ + E_-) + \mathscr{H}\mu_0 m_j \pm \frac{1}{2}\mathscr{H}C\mu_0 \pm \frac{m_j}{2l+1}(E_+ - E_{\ldots})$. Обозначим через E_c энергию центра тяжести уровней в отсутствии поля, т. е.

$$E_c = \frac{E_+(l+1) - E_- l}{2l+1}$$

(статистические веса состояний с E_+и E_-относятся друг к другу как $\left(\frac{2l+1}{2l}\right)$, а через ΔE разность $E_+ - E_-$.В новых обозначениях E будет иметь внд

$$E = E_{\boldsymbol{c}} + \mathscr{H}\mu_0\left(m_j \pm \frac{1}{2}\right) \pm \frac{\Delta E}{2l+1}\left(m_j \mp \frac{1}{2}\right).$$

Это выражение, как легко убедиться, тождественно с выражением задачи 53&7.

Верхний знак соответствует состоянию с $m_l = m_j - 1/2$, $m_s = 1/2$, а нижний-состоянию с $m_l = m_j + 1/2, m_s = 1/2$.

52. $c_1 = \sqrt{\frac{1}{2}(1+\gamma)}$, $c_2 = \sqrt{\frac{1}{2}(1-\gamma)}$ для верхнего

$c_1 = \sqrt{\frac{1}{2}(1-\gamma)}$, $\quad c_2 = -\sqrt{\frac{1}{2}(1+\gamma)}$ для ниж-

где

$$\gamma = \frac{\frac{1}{2}\Delta E + \frac{m_j}{2l+1}\mathscr{H}\mu_0}{\sqrt{\frac{1}{4}(\Delta E)^2 + \frac{m_j}{2l+1}\Delta E\mathscr{H}\mu_0 + \frac{1}{4}\mathscr{H}^2\mu_0^2}}.$$

Нсследуем предельные случаи.

а) Магнитное поле исчезаюие мало, т. е. $\Delta E \gg\gg \mu_0$, тогда $\gamma \approx 1$. Для верхнего уровня будем иметь $c_1 = 1$, $c_2 = 0$, для нижнего $c_1 = 0, c_2 = 1$.

б) Сильное магнитное поле $\triangle E \ll \mathcal{H}_{\mu_0}$ В этом случае $\gamma = \frac{m_j}{l-\frac{1}{2}}$

$$c_1 = \sqrt{\frac{l+m_j+\frac{1}{2}}{2l+1}}, \quad c_2 = \sqrt{\frac{l-m_j+\frac{1}{2}}{2l+1}} \text{ для верхнего}$$

Подставляя полученные значения c_1 и c_2 в выражение пля волновых функций, находим:

$$\psi = R_{nl}^{(0)} \begin{pmatrix} Y_{l,m-1j_2}(\theta,\varphi) \\ 0 \end{pmatrix} \text{ для верхнего уровня,}$$

$$\psi = R_{nl}^{(0)} \begin{pmatrix} 0 \\ Y_{l,m-1,2}(\hat{\varphi},\varphi) \end{pmatrix} \text{ Д.я нижнего уровня.}$$

1+52

Так как энергия в магнитном поле значительно превышает энергию спин-орбитального взаимодействия, то в первом приближении последним взаимодействием пренебрежем.

В этом случае $\hat{l}_z$ и $\hat{s}_z$ - величины сохраняючиеся, и энергия расшепления определяется формулой

$$E^{(1)} = \frac{e\hbar}{2\mu c} e^{\gamma}(m_l + 2m_{\mathrm{s}}).$$

Во втором приближении учтем спин-орбитальное взаимодействие. Мультиплетное расщепление, накладываемое на расщепление в магнитном поле, определится средним значением оператора $\frac{e^2}{2\mu^2c^2}\frac{1}{r^3}(\hat{l}\hat{s})$ (см. задачу 10§7) по состоянию с данными значениями m_l и m_s. При заданном значении одной из компонент момента средние значения двух других равны нулю, поэтому

$$\bar{\vec{l}\hat{s}} = m_l m_s.$$

Таким образом, энергия расщепления уровней с учетом с пин-орбитального взаимодействия имеет вид

$$E^{(1)} = \frac{e\hbar}{2\mu c}\mathscr{H}(m_l + 2m_s) + \frac{e^2\hbar^2}{2\mu^2c^2}\overline{\frac{1}{r^3}} m_l m_{s\circ}$$

Подставим в полученную формулу значение $\overline{\frac{1}{r^3}}$, выраженное через энергию расщепления тонкой структуры в отсутствии поля. Как легко показать (см. задачу 10$7).

$$\frac{e^2\hbar^2}{2\mu^2c^2}\overline{\frac{1}{r^3}} = \frac{E_{n,l,j=l+1,2} - E_{n,l,j=l-1,2}}{l+\frac{1}{2}} = \frac{\Delta E}{l+\frac{1}{2}}.$$

Окончательно для $E^{(1)}$ имеем выражение

$$E^{(1)} = \frac{e\hbar}{2\mu c} e^{\mathcal{H}}(m_l + 2m_s) + \frac{\Delta E}{l+\frac{1}{2}} m_l m_s$$

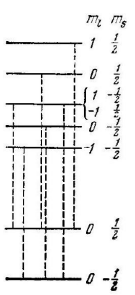


Рис. 30.

На рисунке 30 дана схема расщепления $1s$ и $2p$ термов атома щелочного металла в сильном магнитном поле.

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Энергия возмущения в данном случае равна

$$\hat{V} = \frac{e\hbar}{\mu c}\beta\frac{1}{r^3}\hat{i}\left\{\frac{3(r\hat{s})r}{r^2} - \hat{s}\right\} + \frac{e\hbar}{\mu c}\mathscr{H}\hat{s}_z + \beta\mathscr{H}\hat{i}_z$$

В этом выражении последним членом пренебрежем ввиду малости магнитного момента ядра по сравнению с магнитным моментом электрона $\left(\beta < \frac{e\hbar}{2\mu c}\right)$. Поступая так же, как и при решении задачи 51&7, находим секулярное уравнение:

$$\begin{vmatrix} E_+ + \frac{\mu_0 \mathscr{H} m_f}{i+\frac{1}{2}} - E & \frac{\mathscr{H}\mu_0}{i+\frac{1}{2}}\sqrt{\left(i+\frac{1}{2}\right)^2 - m_f^2} \\ \frac{\mathscr{H}\mu_0}{i+\frac{1}{2}}\sqrt{\left(i+\frac{1}{2}\right)^2 - m_f^2} & E_- - \frac{\mathscr{H}\mu_0}{i+\frac{1}{2}}m_f - E \end{vmatrix} = 0.$$

Здесь E_+и E_-- энергия терма с учетом сверхтонкой структуры, причем E_+относится к состоянию с $f = i + 1/z$, а E_-с $f = i - 1/2, m_f$ проекция полного момента ($m_f = f,\ f-1, ..., -f$), а $\mu_0 = \frac{e\hbar}{2\mu c}$. Решая секулярное уравнение, находим:

$$E = \frac{E_+ + E_-}{2} \pm \frac{\Delta E}{2}\sqrt{1 + \frac{2\xi}{i+\frac{1}{2}}m_f + \xi^2}$$

где $\Delta E = E_+ \cdots E_-$, а $\xi = \frac{2\mu_0\theta}{\Delta E}$.

Найдем поряпок величины напряженности магнитного поля, в котором будет наблюдаться расщепление, описываемое полученной формулой. По условию $\mathcal{F}' \sim \frac{|\Delta E_{ff'}|}{\mu_0}$. В случае атома натрия $\Delta E_{ff'} = 0,0583cM^{-1} = 1,962 \cdot 10^{-16}\partial p2$; так как $\mu_0 = 0,922 \cdot 10^{-20}$ ааусс $\cdot cM^3$, то напряженность ё по порядку должна быть равна $\mathscr{H} \sim 600$ гаусс.

Рассмотрим предельные случаи.

а) В случае малых полей, т. е. при $\mu_0 \rightleftharpoons \mathcal{H} \ll \Delta E$, пля энергии получаем следующие выражения:

$$E = E_+ + \frac{\mathscr{O}\mu_0}{i+\frac{1}{2}}m_f,$$
$$E = E_- - \frac{\mathscr{H}\mu_0}{i+\frac{1}{2}}m_f.$$

б) В случае больших полей, т. е. при е $\mu_0 \gg \Delta E$,

$$E = \frac{1}{2}(E_+ + E_-) \pm \mathscr{H}\ell\mu_0.$$

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Собственные нормированные функции атома водорода в невозмущенном состоянии имеют вид (см. задачу 20 §4)

$$\left.\begin{aligned} \psi_{nlj=l+1/2\,m_j} &= \frac{R_{n,j-1/2}}{\sqrt{2j}}\begin{pmatrix}\sqrt{j+m_j}\,Y_{j-1/2,\,m_j-1/2} \\ \sqrt{j-m_j}\,Y_{j-1/2,\,m_j+1/2}\end{pmatrix} = u_-, \\ \psi_{nlj=l-1/2\,m_j} &= \frac{R_{n,j+1/2}}{\sqrt{2j+2}}\begin{pmatrix}\sqrt{j+1-m_j}\,Y_{j+1/2,\,m_j-1/2} \\ -\sqrt{j+1+m_j}\,Y_{j+1/2,\,m_j+1/2}\end{pmatrix} = u_+. \end{aligned}\right\}$$

Энергия определяется двумя квантовыми числами n, j. В присутствии однородного элекгрического поля $(\mathscr{E}_x = \mathscr{E}_y = 0,\ \mathscr{G}_z = \})\,\hat{j}_z$ по-прежнему остается константой движения, а орбитальный момент перестает быть интегралом движения. Матричные элементы оператора возмущения $\hat{V} = e\&z$ для переходов между состояниями с различными значениями m_j равны нулю. Равны нулю также диагональные элементы оператора $\hat{V}$, т. е.

$$\sum_\sigma \int u_+^* z u_+ d\tau = \sum_\sigma \int u_-^* z u_- d\tau.$$

Поэтому для определения расщепления необходимо вычислить матричные элементы $\hat{V}$, соответствующие переходу из состояния $n, j, m_j, l = j + 1/2$ в состояние $n, j, m_j,\ l = j - 1/2$. Искомый матричный элемент равен

$$V_{21} = V_{12} = e\mathscr{G} \sum_{\sigma} \int u_-^* z u_+ d\tau =$$

$$= \int_0^\infty r^8 R_{n,j-1/2}(r) R_{n,j+1/2}(r) dr \frac{1}{2\sqrt{j(j+1)}} \times \left\{ \sqrt{(j+m_j)\,(j-m_j+1)} \times \right.$$

$$\left. \times \int Y^*_{j-1/2,m_j-1/2} Y_{j+1/2,m_j-1/2} \cos\vartheta dQ - \sqrt{(j-m_j)\,(j+m_j+1)} \times \int Y^*_{j-1/2,m_j+1/2} Y_{j+1/2,2,m_j+1/2} \cos\vartheta dQ \right\}.$$

Проинтегрируем сперва по углам. На основании формулы

$$\cos 0 Y_{lm}(i,\varphi) = \sqrt{\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}} Y_{l+1,m}(\theta,\varphi) + \sqrt{\frac{(l+m)(l-m)}{(2l+1)(2l-1)}} Y_{l-1,m}(\theta,\varphi)$$

получаем, что выражение в фигурной скобке в (3) равно

$$\frac{1}{2\sqrt{j(j+1)}} \{(j+m_j)\,(j-m_j+1) - (j+m_j+1)\,(j-m_j)\} = \frac{m_j}{\sqrt{j(j+1)}}.$$

Производя далее интегрирование по r, имеем:

$$-\frac{3}{2} n \sqrt{n^2 - \left(j+\frac{1}{2}\right)^2}.$$

Таким образом, для матричного элемента возмущения (3) окончательно получаем:

$$-\frac{3}{4} n \frac{\sqrt{n^2 - \left(j+\frac{1}{2}\right)^2}}{j(j+1)} m_j e\mathcal{G} = V_{12} = V_{21}.$$

Искомую поправку к энергии находим из решения векового уравнения:

$$\begin{vmatrix} -\varepsilon & V_{12} \\ V_{21} & -\varepsilon \end{vmatrix} = 0, \quad \varepsilon = \pm V_{12},$$

$$\varepsilon = \pm \frac{3}{4} \sqrt{n^2 - \left(j+\frac{1}{2}\right)^2} \frac{n m_j}{j(j+1)} e\varepsilon.$$

При заданном n терм с $j = n - 1/2$ в электрическом поле не расщепляется, так как он не вырожден относительно квантового числа l (l имеет фиксированное значение $l = j - 1/2 = n - 1$). Все остальные термы тонкой структуры распадаются на $2j + 1$ равноотстоящих уровней $m_j = -j, \ldots \cdot \ldots + j$) 58.

$$\mu_0 = \frac{e\hbar}{2\mu c} \frac{\left(j+\frac{1}{2}\right)^2}{j(j+1)} m_j.$$

1+58

В рассматриваемом случае спин-орбитальное взаимодействие V_1, релятивистская поправка на изменение массы V_2 и энергия электрона во внешнем однородном электрическом поле $V_3 = -Fz$ величины одного и того же порядка. Поэтому мы будем рассматривать их сумму как малое возмущение исходной системы. При вычислении исходим из состояний, в которых имеют вполне определенные значения орбитальный момент L, его проекция m_l и проекция спина m_s на направление электрического поля (ось z).

Вычисляя матричные элементы величин V_1, V_2 и V_3, имеем (в ат. ед.):

$$(V_1)^{l'm'_l}_{lm_l} = \begin{cases} \frac{1}{2}\alpha^2 \frac{m_l(m-m_l)}{n^3 l\left(l+\frac{1}{2}\right)(l+1)}\delta_{nl'} & \text{при } m'_l = m_l, \\ \frac{1}{4}\alpha^2 \frac{\sqrt{\left(l+\frac{1}{2}\right)^2 - m^2}}{n^3 l\left(l+\frac{1}{2}\right)(l+1)}\delta_{ll'} & \text{при } m'_l = m + \frac{1}{2}, \\ m_l = m - \frac{1}{2} \text{ или наоборот}, \\ 0 \quad \text{во всех остальных случаях}, \end{cases}$$

$$(V_2)^{i_l m'_l}_{lm_l} = -\frac{1}{2}\frac{a^2}{n^3}\left(\frac{1}{l+\frac{1}{2}} - \frac{3}{4n}\right)\delta_{ll'}\delta_{ml^m l'}{}'$$

$$(V_3)^{l'm'_l}_{lm_l} = -\frac{3n}{2}\sqrt{\frac{\left(n^2-l^2\right)\left(l^2-m_l^2\right)}{4l^2-1}}F\delta_{l',l-1}\delta_{ml''l}.$$

В случае $n = 2$ энергия состояний с квантовыми числами $l = 1, m = m_l + m_s = \pm 3/2 (j = 3/2)$ в электрическом поле не изменяется. Смещение этого уровня вследствие учета V_1 и V_2 равно $\frac{a^2}{128}$ ат. ед. (см. задачу 10§7).

Расщепление уровня, квантовые числа которого $n = 2, m = \pm\frac{1}{2}$, находится из решения секулярного уравнения

$$\begin{vmatrix} -\frac{11}{4}\delta - E^{(1)} & \delta\sqrt{2} & 0 \\ \delta\sqrt{2} & -\frac{7}{4}\delta - E^{(1)} & -3F \\ 0 & -3F & -\frac{15}{4}\delta - E^{(1)} \end{vmatrix} = 0,$$

где $3\delta = \frac{\alpha^2}{32}$ ат. ед. есть расщепление тонкой структуры уровня $n = 2$ в отсутствии внешнего поля. Введем в это уравнение величину ε, связанную с $E^{(1)}$ соотношением $E^{(1)} = \varepsilon - \frac{11}{4}\delta$ $\left(-\frac{11}{4}\delta\right.$ представляет энергию центра тяжести трех энергетических уровней $\left.\frac{E_1^{(1)}+E_2^{(1)}+E_3^{(1)}}{3} = -\frac{11}{4}\delta\right)$, получаем:

$$\begin{vmatrix} -\varepsilon & \delta\sqrt{2} & 0 \\ \delta\sqrt{2} & \delta - \varepsilon & -3F \\ 0 & -3F & -\delta - \varepsilon \end{vmatrix} = 0,$$

или

$$\varepsilon^3 - \varepsilon\left(3\delta^2 + 9F^2\right) - 2\partial^3 = 0.$$

Решаем последнее уравнение в случае слабых полей ($F \ll \delta$) и в случае сильных полей ($F \gg$ о). В первом случае получаем:

Во втором:

$$\varepsilon_1 = -\delta - \sqrt{3}F - \frac{F^2}{\delta}$$
$$\varepsilon_2 = -\delta + \sqrt{3}F - \frac{F^2}{\delta},$$
$$\varepsilon_3 = 2\delta + 2\frac{F^2}{\delta}$$
$$\varepsilon_1 = -3F - \frac{1}{2}\frac{\delta^2}{F} + \frac{1}{9}\frac{\delta^3}{F^2},$$
$$\varepsilon_2 = -\frac{2}{9}\frac{\delta^3}{F^2},$$
$$\varepsilon_3 = 3F + \frac{1}{2}\frac{\delta^2}{F} + \frac{1}{9}\frac{\delta^3}{F^2}$$

1+59

Среднее значение полной энергии равно

$$\hat{H} = \frac{\int \psi_0^*(1+\lambda u)\hat{H}\psi_0(1+\lambda u)d\tau}{\int \psi_0^*\psi_0(1+\lambda u)^2 d\tau}.$$

С помощью интегрирования по частям приведем числитель к более удобной форме.

Оператор кинетической энергии электронов имеет вид

$$\hat{T} = -\frac{1}{2}\sum_{i=1}^{n}\Delta_i,$$

где n-число электронов, а Δ_i - оператор Лапласа, действующий на координаты i-го электрона. (Расчет производим в атомной системе единиц.) Запишем выражение для среднего значения кинетической энергии в симметричной относительно «0 и Чо форме

$$\overline{\hat{T}} = -\frac{1}{2}\sum_{i=1}^{n}\frac{1}{2}\int\{\psi_0^*(1+\lambda u)\Delta_i(1+\lambda u)\psi_0 + \\ +\psi_0(1+\lambda u)\Delta_i(1+\lambda u)\psi_0^*\}\,d\tau.$$

Выполняя дифференцирование под знаком интеграла, получим:

$$\overline{\hat{T}} = -\frac{1}{2}\sum_{i=1}^{n}\frac{1}{2}\int\{\psi_0^*(1+\lambda u)^2\Delta_i\psi_0 + \\ +\psi_0(1+\lambda u)^2\Delta_i\psi_0^* + 2\lambda\psi_\psi\psi_0^*(1+\lambda u)\Delta_i u + \\ +2\lambda(1+\lambda u)\nabla_i\left(\psi_0^*\psi_0\right)\nabla_i u\}\,d\tau.$$

Преобразуем два последние члена. Для этого рассмотрим тождество

$$\nabla_i\{\psi_{0'}^*\langle(1+\lambda u)\nabla_i u\} = \\ = \psi_{\sigma''0}^*(1+\lambda u)\Delta_i u + (1+\lambda a)\nabla_i\left(\psi_0^*\psi_0\right)\nabla_i u + \lambda\psi_0^*\psi_0\left(\nabla_i u\right)^2.$$

При интегрировании тождества (3) по всему конфигурационному пространству имеем:

$$\int\{\psi_0^*\psi_0^*(1+\lambda.u)\Delta_i u + (1+\lambda u)\nabla_i\left(\psi_0^*\psi_0\right)\nabla_i u\}\,d\tau = \\ = -\lambda\int\psi_0^*\left(\nabla_i u\right)^2 d\tau.$$

Подставляя (4) в (2), получим:

$$\overline{\hat{T}} = -\tfrac{1}{2}\sum_{i=1}^{n}\tfrac{1}{2}\int\left\{\psi_0^*(1+\lambda u)^2\Delta_{i\psi_0} + \psi_0(1+\lambda u)^2\Delta_i\psi_0^*\right\}d\tau + \\ +\tfrac{\lambda 2}{2}\sum_{i=1}^{n}\int_0\psi_0^*\psi_0\left(\nabla_i u\right)^2 d\tau.$$

Оператор Гамильтона $\hat{H}$ равен $\hat{H} = \hat{H}_0 + u = \hat{T} + \hat{V} + u$. Учитывая коммутативность $\hat{V}$с$(1+\lambda u)$, выражение (1) представим в следующей форме:

$$\overline{\hat{H}} = E_0 + \frac{\frac{1}{2}\int(1+\lambda u)^2\left(\psi_0^*\hat{H}\Psi_0 + \iota_0\hat{H}_{\iota_0^*}^*\right)d\tau + \frac{\lambda^2}{2}\sum_{i=1}^{n}\int\bigcup_0^*\psi_0\left(\nabla_i u\right)^2 d\tau}{\int(1+\lambda u)^2\iota_0^*\psi_0 d\tau}.$$

Так как $\hat{H}_0\psi_0 = E_0\iota_0$, то
Или

$$\overline{\hat{H}} = E_0 + \frac{\int\psi_0^* u(1+\lambda u)^2\psi_0 d\tau + \frac{\lambda^2}{2}\sum_{i=1}^{n}\int\psi_0^*\psi_0\left(\nabla_i u\right)^2 d\tau}{\int(1+\lambda u)^2\psi_0^*\psi_0 d\tau}$$

$$(u)_{00} + 2\lambda\left(u^2\right)_{00} + \lambda^2\left(u^3\right)_{00} + \frac{\lambda^2}{2}\sum_{i=1}^{n}\left\{\left(\nabla_i u\right)^2\right\}_{00}$$

где $(u)_{00} = \int\psi_0^* u_0 d\tau$, $\left(u^2\right)_{00} = \int\psi_0^* u^2\psi_0 d\tau$ и т. д. Разложим второй член в (5) в ряд, отбросив члены с $\left(u^3\right)_{00}, (u)_{00}^3$ и т. д.
Для добавки к энергии ΔE получим приближенное выражение вида

$$\Delta E \approx (u)_{00} + 2\lambda\left(u^2\right)_{00} - 2\lambda(u)_{00}^2 + \frac{\lambda^2}{2}\sum_{i=1}^{n}\left\{\left(\nabla_i u\right)^2\right\}_{00}.$$

Определим значение вариационного параметра λ из условия

$$\frac{d\Delta E}{d\lambda} = 2\left(u^2\right)_{00} - 2(u)_{00}^2 + \lambda\sum_{i=1}^{n}\left\{\left(\nabla_i u\right)^2\right\}_{00} = 0,$$

$$\bar{\hat{H}} = E_0 + \frac{\overbrace{i=1}}{1 + 2\lambda\,(u)_{00} + \lambda^2\,(u^2)_{00}},$$

откуда для λ получаем значение

$$\lambda = 2\frac{(u)_{00}^2 - \left(u^2\right)_{00}}{\sum\limits_{i=1}^{n}\left\{\left(\nabla_i u\right)^2\right\}_{00}}$$

Подставляя λ в (6), получим искомое соотношение

$$\Delta E \approx (u)_{00} - 2\frac{\left\{(u)_{00}^2 - \left(u^2\right)_0\right\}^2}{\sum\limits_{i=1}^{n}\left\{\left(\nabla_i u\right)^2\right\}_{00}}$$

1+60

Если атом находится в однородном электрическом поле, напряженность которого &, и поле направлено по оси z, то оператор возмущения

$$u = -\& \sum_{i=1}^{n} z_i = -\mathcal{E}z.$$

Матричный элемент $(u)_{00}$ равен нулю.
На основании формулы (7) предыдущей задачи имеем

$$\Delta E \approx -2\xi^2 \frac{\left\{\left(z^2\right)_{00}\right\}}{n},$$

где n-число электронов.
Отсюда следует, что коэффициент поляризуемости равен

$$\alpha = \frac{4\left\{\left(z^2\right)_{00}\right\}^2}{n}.$$

Необходимо отметить, что эта формула, полученная путем введения только одного вариационного параметра λ, представляет удовлетворительное приближение лишь для атома водорода и гелия. В случае атомов с несколькими электронными оболочками деформации оболочек будут не одинаковы. Следовательно, в вариационном методе для получения более удовлетворительного результата мы должны для каждой электронной оболочки ввести свой вариационный параметр λ
Для атома водорода

$$\left(z^2\right)_{00} = \frac{1}{3}\left(r^2\right)_{00} = \frac{1}{3}\frac{4\pi}{\pi}\int_0^\infty e^{-2rr^4}dr = 1$$

и, следовательно, $\alpha = 4$ ат. ед.
В системе CGSE $\alpha = 4\left(\frac{\hbar^2}{\mu e^2}\right)cM^3$.

Для атома гелия волновую функцию основного состояния возьмем в виде

$\psi_0 = \frac{Z_{эфф}^3}{\pi} e^{-Z_{эфф}(r_1+r_2)}$, где $Z_{эфф} = \frac{27}{16}$ (см. задачу 14 § 7).

Произведя вычисления, получим:

$$\alpha = 0,98 \text{ ат. ед. или } \alpha = 0,98\left(\frac{\hbar^2}{\mu e^2}\right)^3 \text{ с. }^3.$$

Для найденного значения α величина диэлектрической постоянной гелия при нормальных условиях будет равна

$$\varepsilon = 1,00049.$$

Экспериментальное значение $\varepsilon_{эксп} = 1{,}00074$.

Сравнительно большое различие между вычисленным значением и экспериментальным объясняется главным образом тем, что мы пользовались грубой аппроксимацией для невозмущенной функции.

1+61

а)

$$E^{(1)} = \frac{m_j}{8j(j+1)} \frac{e\hbar}{\mu c} \{(2j+1)^2 \mathscr{H} \pm$$

$$\pm \sqrt{(2j+1)^2 e^{2c^2} + \frac{36n^2}{\alpha^2} \left\{ n^2 - \left(j + \frac{1}{2} \right)^2 \right\}}]^2$$

$$\left(\alpha = \frac{e^2}{\hbar c} \right)$$

(см. задачи 57, 59$7);
6.

$$E^{(1)} \left(n = 2, m_j = \pm \frac{3}{2} \right) = -\frac{\alpha^2}{128} \left(\frac{\mu e^4}{\hbar^2} \right) \pm \frac{e\hbar}{\mu c} \tilde{f}_t,$$

$$E^{(1)} \left(n = 2, m_j = \pm \frac{1}{2} \right) = \varepsilon - \frac{11}{384} \alpha^2 \left(\frac{\mu e^4}{\hbar^2} \right),$$

где e определяется из решения уравнения третьей степени

$$\varepsilon^3 \mp 2\beta\varepsilon^2 - \varepsilon \left(3\delta^2 + 9F^2 - \beta^2 \right) \pm 2\delta^2\beta - 2\delta^3 = 0.$$

Здесь $\beta = \frac{e\hbar}{2\mu c} \mathscr{H}$, $F = e\mathscr{E} \left(\frac{\hbar^2}{\mu e^3} \right)$, $\delta = \frac{\alpha^2}{96} \left(\frac{\mu e^4}{\hbar^2} \right)$.

В случае сильных полей ($\delta \ll F\delta \ll \beta$)

$$\varepsilon_1 = \pm\beta - 3F - \frac{1}{2} \frac{9F \mp \beta}{9F^2 \mp 3F\beta} \delta^2,$$

$$\varepsilon_2 = \pm \frac{2\beta}{9F^2 - \beta^2} \delta^2,$$

$$\varepsilon_3 = \pm\beta + 3F + \frac{1}{2} \frac{9F \pm \beta}{9F \pm 3F\beta} \delta^2$$

(см. задачу 59§7).

1+62

Направим ось z вдоль направления магнитного поля, а ось x вдоль электрического поля. Тогда для оператора потенциальной энергии электрона в этих полях получим

$$w = \frac{e\hbar}{2\mu c} (\hat{l}_z + 2\hat{s}_z) \mathscr{H} + e\mathscr{E}x.$$

Последнее выражение будем рассматривать как малое возмущение, характеризуя невозмущенное стационарное состояние квантовыми числами $n, l, m, \sigma (m$ и 5 - проекции орбитального и спинового моментов на ось $z)$. Отличные от нуля матричные элементы x имеют вид

$$(x)^{l-1,m}_{l,m-1} = (x)^{l,m-1}_{l-1,m} = \frac{3}{4} n \sqrt{\frac{(n^2 - l^2)(l - m + 1)(l - m)}{(2l+1)(2l-1)}} a,$$

$$(x)^{l,m}_{l-1,m-1} = (x)^{l-1,m-1}_{l,m} = -\frac{3}{4} n \sqrt{\frac{(n^2 - l^2)(l + m - 1)(l + m)}{(2l+1)(2l-1)}} a$$

$$\left(a = \frac{h^2}{\mu, e^2} \right).$$

Рассмотрим случай $n = 2$. Пусть для определенности проекция спина на ось z равна $+1/2$. Введем обозначения $\beta = \frac{eh}{2\mu.c}$ ef, $\gamma = \frac{3}{\sqrt{2}} e\&a$. Матрица оператора возмущения в этих обозначениях имеет следующий вид:

$$\begin{pmatrix} 2\beta & 0 & 0 & -\gamma \\ 0 & \beta & 0 & 0 \\ 0 & 0 & 0 & \gamma \\ -\gamma & 0 & \gamma & \beta \end{pmatrix}.$$

Нумерация состояний производится в порядке убывания l и m. Состояние с квантовыми числами $l = 1, m = 0$ не комбинирует с остальными. Энергия этого состояния равна $E_1^{(1)} =$ з. Остальные три собственные значения матрицы возмущения находятся из решения секулярного уравнения

$$E^3 - 3\beta E^2 + 2\left(\beta^2 - \gamma^2\right) E + 2\gamma^2\beta = 0.$$

Решая его, имеем:

$$E_2^{(1)} = \beta, E_{3,4}^{(1)} = \beta \pm \sqrt{3^2 + 2\gamma^2}$$

или, подставляя значения & и γ,

$$E_2^{(1)} = \frac{e\hbar}{2\mu c}\mathscr{H}, E_{3,4}^{(1)} = \frac{e\hbar}{2\mu c}\left\{\mathscr{H} \pm \sqrt{\mathscr{H}^2 + \frac{36}{\alpha^2}g^2}\right\}.$$

18.1.11 Basic problems about molecules

Б-2.11.8 Основное состояние по правилу Хунда

Пользуясь правилами Хунда, определить значения квантовых чисел L, S и J в основных состояниях следующих атомов:
а) кремния, б) фосфора, в) серы, г) ванадия, д) кобальта, е) церия.
Для случаев а), б) и в) найти все термы. Записать спектроскопические символы полученных состояний.

Solution

Суть решения в том, что
Для первого порядка теории возмущений первое правило Хунда гласит: энергия атома имеет минимальное значения в состояниях с максимально возможным значением полного спина S. Если при этом возможны несколько различных значений полного орбитального момента, минимальную энергию имеют состояния с максимальным значением L.
Для второго порядка теории возмущений формулируется второе правило Хунда: минимальную энергию имеет терм с $J = |L - S|$, если электронная оболочка заполнена меньше, чем наполовину, и с $J = L + S$ в противном случае.
(подумаю потом про это)
Приводим ответы, в электронных конфигурациях указаны только электроны на незаполненных оболочках.

Атом	Конфигурация	Возможные термы	Нормальный терм
$_{14}$Si	$3s^2 3p^2$	${}^1S_0, {}^1D_2, {}^3P_0, {}^3P_1, {}^3P_2$	${}^3P_0$
$_{15}$P	$3s^2 3p^3$	${}^4S_{3/2}, {}^2P_{1/2}, {}^2P_{3/2}, {}^2D_{3/2}, {}^2D_{5/2}$	${}^4S_{3/2}$
$_{16}$ S	$3s^2 3p^4$	${}^1S_0, {}^1D_2, {}^3P_0, {}^3P_1, {}^3P_2$	${}^3P_2$
$_{23}$ V	$3d^3 4s^2$		${}^4F_{3/2}$
$_{27}$Co	$3d^7 4s^2$		${}^4F_{9/2}$
$_{58}$Ce	$4f5d6s^2$		${}^1G_4\left({}^3H_4\right)$

Элемент Ce представляет собой одно из немногих исключений из правила Хунда. В скобках записан терм, определенный согласно правилам Хунда (отличающийся от истинного).

МФТИ.кр-?. Основное состояние углерода, азота, кислорода.

Пользуясь правилами Хунда, определите термы основного состояния атомов:
а) углерода, б) азота, в) кислорода.

Solution

Суть решения в том, что

Б-2.11.9 Взаимодействие атома с ионом и атома с атомом

С помощью второго приближения теории возмущений определить зависимость от расстояния R энергии взаимодействия систем:
а) атом + ион;
б) атом + атом.
В обоих случаях атом находятся в S-состоянии.

Формализм решения

При исследовании взаимодействия составных частиц таких, как атомы, с другими атомами или ионами можно использовать теорию возмущений, рассматривая изолированные атом и ион (или другой атом), как невозмущенную систему, а потенциальную энергию их электростатического взаимодействия - как оператор возмущения. Поскольку скорости относительного движения атомов невелики, мы можем считать, что ядра атомов (ионов) покоятся (приближение Борна-Оппенгеймера).

Считая, что составные частицы находятся на большом расстоянии друг от друга по сравнению с их размерами ($r_a \ll R$), найдем энергию их электрического взаимодействия в виде разложения по степеням $1/R$. Первый неисчезающий член такого разложения (в силу электронейтральности атома) дает оператор возмущения нашей задачи:

$$\hat{\boldsymbol{V}} = -\hat{\boldsymbol{d}}\boldsymbol{E},$$

где $\hat{\mathbf{d}}$ - дипольный момент атома, $\mathcal{E}$ - внешнее электрическое поле (при $r_a \ll R$ его можно считать приблизительно однородным на расстояниях $\sim r_a$).

Применим теорию возмущений.

а) Поиск энергии взаимодействия атома и иона

Поле иона - это поле заряженной частицы $\mathcal{E} = Ze\mathbf{R}/R^3$, где Ze - заряд иона. Поэтому оператор возмущения равен:

$$\hat{\mathrm{V}} = -\frac{Ze}{R^3}(\hat{\mathbf{d}}\mathbf{R}) = -\frac{Ze}{R^2}\hat{\mathrm{d}}_z,$$

где $\hat{\mathbf{d}}_z = \sum\limits_a e_a z_a$, и мы считаем, что $\mathbf{R}||Oz$. Поправка первого приближения теории возмущений

$$E^{(1)} = \langle\psi^{(0)}|\hat{V}|\psi^{(0)}\rangle = 0$$

в силу сферической симметрии S-состояний.

Во втором порядке теории возмущений имеем

$$E^{(2)} = \sum_{n,m\neq 0} \frac{|\langle 00|\hat{\mathrm{V}}|nm\rangle|^2}{E_{00}^{(0)} - E_{nm}^{(0)}},$$

где индексы 00 относятся к S-состояниям атома и иона (наинизшим по энергии), индексы n, m нумеруют их возбужденные состояния. Из формулы для $E^{(2)}$ ясно, что $E^{(2)} < 0$, а также $E^{(2)} \sim 1/R^4$, и в итоге получаем общее выражение для потенциала взаимодействия в виде

$$U(R) = E^{(2)} = -\frac{C}{R^4}, \text{ где } C = \text{ const.}$$

Взаимодействие такого типа называется поляризационным.

б) Поиск энергии взаимодействия атома и атома

В этом случае, учитывая, что напряженность электрического поля для атома с дипольным моментом $\hat{\mathbf{d}}_1$ имеет вид $\mathcal{E} = \left[3\left(\hat{\mathbf{d}}_1\mathbf{n}\right)\mathbf{n} - \hat{\mathbf{d}}_1\right]/R^3$, где $\mathbf{n} = \mathbf{R}/R$, из (1) получаем оператор возмущения

$$\hat{\mathrm{V}} = \frac{\left(\hat{\mathbf{d}}_1\hat{\mathbf{d}}_2\right) - 3\left(\hat{\mathbf{d}}_|\mathbf{n}\right)\left(\hat{\mathbf{d}}_2\mathbf{n}\right)}{R^3} = \frac{1}{R^3}\left(\hat{\mathrm{d}}_{x1}\hat{\mathrm{d}}_{x2} + \hat{\mathrm{d}}_{y1}\hat{\mathrm{d}}_{y2} - 2\hat{\mathrm{d}}_{z1}\hat{\mathrm{d}}_{z2}\right).$$

(см. задачу 1.6.7). Аналогично п. а) имеем $E^{(1)} = 0$, а вычисление поправок второго приближения дает

$$U(R) = -\frac{C}{R^6}, \text{ где } C = \text{ const }.$$

Именно такой зависимостью энергии от расстояния характеризуются силы притяжения Ван-дер-Ваальса.

О решении задачи методами КТП (???)

(??? а если считать атомы полями, то как тогда будет их взаимодействие обобщаться??? мб потом подумаю, когда умным стану.)

Б-2.11.10 Дублет натрия в магнитном поле (!?!??)

Желтый дублет атома натрия соответствует оптическим переходам ${}^2P_{3/2} \to {}^2S_{1/2}$; ${}^2P_{1/2} \to {}^2S_{1/2}$. Определить расщепление этого дублета в слабом и сильном магнитном полях. Сравнить полученные картины расщепления линий натрия с расщеплением синглетной линии кадмия, отвечающей переходу ${}^1D \to {}^1P$.

Суть решения и результаты (!!!)

Формализм решения

Гамильтониан атома, находящегося в однородном магнитном поле $\mathcal{H}$, имеет вид

$$\hat{\mathrm{H}} = \frac{1}{2m}\sum_a \left(\hat{\mathbf{p}}_a + \frac{e}{c}\mathbf{A}\left(\mathbf{r}_a\right)\right)^2 + U + \frac{e\hbar}{mc}\mathcal{H}\hat{\mathbf{S}},$$

где $(-e) < 0$ - заряд электрона, суммирование производится по всем электронам атома, U - энергия взаимодействия электронов с ядром и друг с другом, $\hat{\mathbf{S}} = \sum_a \hat{\mathbf{s}}_a$ - оператор суммарного спина электронов. Проводя стандартные преобразования (в частности, выбирая векторпотенциал в виде $\mathbf{A}_u = \frac{1}{2}\left[\mathcal{H}\times\mathbf{r}_a\right]\big)$, получим

$$\hat{\mathrm{H}} = \hat{\mathrm{H}}_0 + \frac{e\hbar}{2mc}\mathcal{H}(\hat{\mathbf{L}} + 2\hat{\mathbf{S}}) + \frac{e^2}{8mc^2}\sum_a \left[\mathcal{H}\times\mathbf{r}_a\right]^2,$$

где $\hat{\mathbf{L}}$ - полный орбитальный момент атома, $\hat{\mathrm{H}}_0$ - гамильтониан атома в отсутствие поля. (!!! в теории обязательно эту формулу укажу, заготовки про нее пока не усвоены!)

Имея в виду дальнейшее рассмотрение задачи по теории возмущений, сделаем ряд приближений, Во-первых, отбросим в (1) член, квадратичный по напряженности поля $\mathcal{H}$, считая, что в достаточно слабом поле он вносит малый вклад в решение по сравнению с линейным по $\mathcal{H}$ слагаемым. Далее, полагая, что поле направлено по оси z, получим $\hat{\mathrm{H}} = \hat{\mathrm{H}}_0 + \hat{\mathrm{V}}_{\mathscr{H}}$, где $\hat{\mathrm{V}}_{\mathscr{H}} = \hbar\Omega\left(\hat{l}_z + 2\hat{\mathrm{S}}_z\right)$ - оператор взаимодействия с магнитным полем, $\Omega = e\mathcal{H}/(2mc)$ - ларморовская частота.

а) Слабое поле

В этом приближении считается, что поправка, связанная с магнитным полем, т. е. $\Delta E_{\mathscr{H}}$, гораздо меньше тонкого расщепления уровней $\Delta E_{\text{тонк}}$ [8)], и поэтому можно применить теорию возмущений к каждому уровню тонкой структуры. При этом оператором возмущения является $\hat{V}_{\mathscr{F}}$, а невозмущенные уровни - это уровни энергии атома с учетом расщепления тонкой структуры, характеризующиеся определенными значениями квантовых чисел L, S, J (т. е. собственными значениями операторов $\hat{\mathbf{L}}^2, \hat{\mathbf{S}}^2, \hat{\mathbf{J}}^2$, где $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$). Правильными векторами нулевого приближения в этом случае являются $|L, S, J, M_J\rangle$ (собственные векторы для операторов $\hat{\mathbf{L}}^2, \hat{\mathbf{S}}^2, \hat{\mathbf{J}}^2, \hat{\mathrm{J}}_z$). Расчет в первом порядке теории возмущений дает

$$\Delta E^{(1)}_{\mathcal{H}} = \hbar\Omega g M_J, \quad \text{где} \quad g = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}$$

есть так называемый фактор Ланде. Отсюда следует, что магнитное поле полностью снимает вырождение по магнитному квантовому числу M_J, каждый уровень тонкой структуры расщепляется на $2J+1$ подуровней.

(??? был вопрос о критерии слабости поля, и какой же он????)

Конкретно для атома натрия находим, что уровень ${}^2P_{3/2}$ расщепляется на четыре компоненты:

$$\Delta E^{(1)}_{2P_{3/2}} = \frac{4}{3}\hbar\Omega M_J, \quad M_J = \pm\frac{1}{2}, \pm\frac{3}{2},$$

а каждый из уровней ${}^2P_{1/2}$ и ${}^2S_{1/2}$ расщепляется на две компоненты:

$$\Delta E^{(1)}_{2P_{1/2}} = \tfrac{2}{3}\hbar\Omega M_J, \quad M_J = \pm\tfrac{1}{2};$$
$$\Delta E^{(1)}_{2S_{1/2}} = 2\hbar\Omega M_J, \quad M_J = \pm\tfrac{1}{2}.$$

Спектр наблюдаемых частот, в соответствии с правилом Бора, имеет вид

$$\omega = \frac{E_2^{(0)} - E_1^{(0)}}{\hbar} + \Omega\left(g_2 M_{/2} - g_1 M_{/1}\right) \equiv \omega_0 + \Delta\omega,$$

причем здесь необходимо учитывать правила отбора для дипольного электрического излучения

$$\Delta J = 0, \pm 1, \qquad \Delta M_J = 0, \pm 1, \qquad \Delta L = \pm 1, \qquad \Delta S = 0.$$

Применяя эти правила, видим, что вместо линии ${}^2P_{3/2} \to {}^2S_{1/2}$ в магнитном поле возникают шесть переходов с частотами (см. (2)) $\Delta\omega = \pm\Omega, \pm\frac{1}{3}\Omega, \pm(5/3)\Omega$, а вместо линии ${}^2P_{1/2} \to {}^2S_{1/2}$ - четыре перехода с частотами $\Delta\omega = \pm(2/3)\Omega, \pm(4/3)\Omega$. Таким образом, в слабом магнитном поле вместо резонансного дублета наблюдается спектр, состоящий из 10 близких спектральных линий (аномальный или сложный эффект Зеемана).

6) Сильное поле.

В данном случае считается, что $\Delta E_{\mathcal{H}} \gg \Delta E_{\text{тонк,}}$, т. е. расщепление в магнитном поле велико по сравнению с интервалами тонкой структуры, но по-прежнему настолько мало, что можно пренебречь квадратичным членом в (1). При этом также можно применить теорию возмущений, но необходимо сначала учесть влияние магнитного поля, а затем (если нужно) - спин-орбитальное взаимодействие, ответственное за тонкую структуру.

Правильными векторами нулевого приближения в данном случае являются $|L, S, M_L, M_S\rangle$, т. е. общие собственные векторы для операторов $\hat{\mathbf{L}}^2, \hat{\mathbf{S}}^2, \hat{l}_z, \hat{\mathrm{S}}_z$. В первом приближении теории возмущений получаем поправку к энергии:

$$\Delta E_{2P}^{(1)} = h\Omega\left(M_L + 2M_S\right)$$

и наблюдаемые частоты (с учетом правила отбора $\Delta M_S = 0$):

$$\omega = \omega_0 + \Omega\Delta M_L, \quad \Delta M_L = 0, \pm 1.$$

Таким образом, в сильном поле наблюдается триплет спектральных линий $\omega_0, \omega_0 \pm \Omega$ (простой или нормальный эффект Зеемана).

В случае кадмия термы ${}^1D$ и ${}^1P$ являются синглетными, т. е. для них $S = 0, J = L$ и, следовательно, $g = 1$. Поэтому независимо от величины напряженности магнитного поля будет наблюдаться простой эффект Зеемана.

Киселев-Л.13.1. Термы углерода (????)

Определить термы и основное состояние атома углерода: конфигурация $1s^2 2s^2 2p^2$

Solution

В этой конфигурации две заполненных s-оболочки, которые не участвуют в определении термов. Пара $2p$-электронов может быть распределена по $2(2l+1)$ состояниям с различными проекциями спина и орбитального момента $l = 1$

$$C_6^2 = \frac{6!}{2!4!} = 15$$

способами.

Максимальное значение спина электронов $S = 1$ является симметричным по перестановкам электронов. Сложение орбитальных моментов электронов $1 + 1$ дает $L = 0, 1, 2$, причем максимальное значение $L = 2$ также является симметричным по перестановкам, значит, оно запрещено для $S = 1$, так как в противном случае состояние было бы симметричным, что противоречит статистике Ферми. Состояние с $L = 0$ также является симметричным по перестановке двух электронов, поэтому оно также запрещено для $S = 1$. В итоге получаем единственный триплетный терм

$${}^3P.$$

Число таких состояний $(2S+1)(2L+1) = 3 \cdot 3 = 9$. При $S = 0$ спиновое состояние является антисимметричным по перестановкам, поэтому допустимы только симметричные орбитальные состояния двух электронов, т. е. $L = 0, 2$. Соответствующие термы

$${}^1S, \quad {}^1D$$

имеют вырождение по проекциям спина и момента

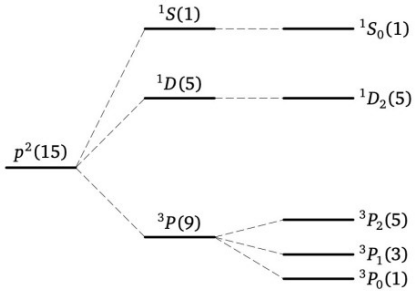
$$1 + 5 = 6.$$

Суммарное число вырождения конфигурации 15 совпадает с суммарным числом состояний термов, которые расщепляются вследствие учета поправок к самосогласованному полю.

Основное состояние согласно правилу Хунда: ${}^3P$.

Приведенное рассуждение является специфическим для двух электронов, поскольку для них за исключением случая заполненной s-оболочки всегда реализуются все состояния, получающиеся сложением орбитальных моментов этих электронов, что, как мы увидим на примере следующей задачи, не имеет места для большего числа эквивалентных электронов, так что приходится использовать наиболее общий метод определения термов.

В атоме углерода основное состояние отвечает терму ${}^3P_0$, а термы ${}^3P_1, {}^3P_2$ находятся последовательно выше согласно правилу интервалов Ланде. Схема расщепления электронной конфигурации углерода при последовательном учете поправок показана на рис. 33.



Киселев-Л.13.2. Термы азота (?????)

Определить термы атома азота: конфигурация $1s^2 2s^2 2p^3$

Solution

Три $2p$-электрона на незаполненной оболочке могут быть распределены по $2(2l+1)$ состояниям с различными проекциями спина и орбитального момента $l = 1$ $C_6^3 = \frac{6!}{3!3!} = 20$ способами.

Максимальное значение спина электронов $S = \frac{3}{2}$ является симметричным по перестановкам электронов, и оно возможно, только если электроны с проекцией полного спина $\frac{3}{2}$ занимают состояния с различными значениями проекции орбитального момента: схема расположения p-электронов с различными проекциями суммарного орбитального момента $m =$ |↑|↑|↑|, а значит, при проекции суммарного орбитального момента только $M = 0$, т. е. исключительно при $L = 0$. Поэтому при максимальном значении спина электронов единственный терм

$${}^4S \mapsto {}^4S_{3/2}.$$

Число таких состояний $(2S+1)(2L+1) = 4 \cdot 1 = 4$.

При $S = \frac{1}{2}$ допустимые значения суммы проекций орбитального момента $M = \pm 2, \pm 1, \pm 0$. Термы с максимальными значениями $|M| = 2$ отвечают $L = 2$:

$${}^2D \mapsto {}^2D_{5/2}, {}^2D_{3/2},$$

и они имеют вырождение по проекциям спина и момента

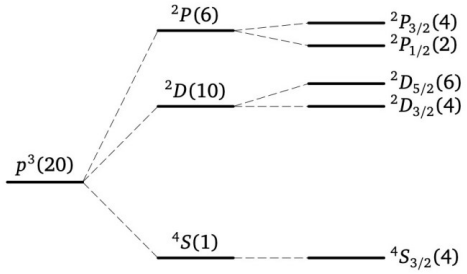
$$2 \cdot 5 = 10, \quad \text{или} \quad \sum_J (2J+1) = 6 + 4 = 10.$$

Состояния с $M_S = +\frac{1}{2}$ и $M = +1$ - это |↑↓| |↑| и |↑|↑↓| |. Одна из суперпозиций отвечает терму с $S = \frac{1}{2}$ и $L = 2$, описанному выше, но просто с другим значением проекции M, а другая, следовательно, терму с $S = \frac{1}{2}$ и $L = 1$. Значит, в конфигурации есть еще и терм

$${}^2P \mapsto {}^2P_{3/2}, {}^2P_{1/2},$$

который имеет вырождение по проекциям спина и орбитального момента $2 \cdot 3 = 6$ или по проекциям полного момента $4 + 2 = 6$.

Состояния с $M_S = +\frac{1}{2}$ и $M = 0$ включают в себя три спин-орбитальных конфигутолько три ортогональных суперпозиции, отвечающих уже найденным нами термам $^2D, ^2P$ и ^4S. Поэтому независимых состояний, отвечающих каким-то новым термам, больше нет. В этом можно убедиться, суммируя количество состояний в термах: $^2D + ^2P + ^4S = 10 + 6 + 4 = 20$, которое исчерпывает степень вырождения конфигурации по проекциям орбитального момента и спина. Основное состояние азота согласно правилам Хунда $-^4S_{3/2}$. Схема расщепления электронной конфигурации азота при последовательном учете поправок показана на рис. 34.



Spaldin-3.2(2 min) Fe^{2+} ion basic properties

In this problem we will calculate the electronic structure and magnetic properties of an important transition-metal ion: Fe^{2+}.

(a) What is the electronic configuration of an Fe^{2+} ion? (Note that the transition metals give up their 4 s electrons before their 3 d electrons on ionization.)

(b) Use Hund's rules to determine the values of S, L, and J in the ground state of an Fe^{2+} ion.

(c) Calculate the Landé g-factor using Eq. (3.28).

(d) Calculate the total magnetic moment of an Fe^{2+} ion, $g\sqrt{J(J+1)}\mu_B$, and the magnetic moment along the field direction, $gM_J\mu_B$. Compare your result with your answer to Exercise 1.3(b).

(e) Try calculating the total magnetic moment using the value of S determined in 3.2(b), but assuming that $L = 0$ (so $J = S$). In fact the measured value is $5.4\mu_B$. More about this later!

(??? задача вроде как простая, да вот нужно подумать про нее еще больше.)

Solution for 3.2(a)

(?????? а я не знаю, откуда это????)

The electronic configuration of an Fe atom is

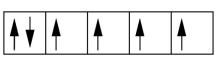
$$(1s)^2(2s)^2(2p)^6(3s)^2(3p)^6(4s)^2(3d)^6$$

Therefore, because the transition elements give up their 4 s electrons before their 3 d electrons on ionization, the electronic configuration of an Fe^{2+} ion is

$$(1s)^2(2s)^2(2p)^6(3s)^2(3p)^6(3d)^6$$

Solution for 3.2(b)

Hund's first rule tells us that the electrons maximize their total spin, S. Therefore they arrange themselves one electron per d orbital with parallel spins before pairing up with opposite spins in the same orbital. For iron, the resulting configuration looks like:



Therefore the total spin, $S = 4 \times \frac{1}{2} = 2$.

The five d orbitals have m_l values of $-2, -1, 0, 1$, and 2. Depending on which d orbital contains two electrons, the total M_L can be $-2, -1, 0, 1$, or 2. Therefore, since $M_L = -L, -L+1, ..., 0, ..., L-1, L$, the total orbital quantum number, L, must be equal to 2.

Finally, from Hund's third rule, because the shell is more than half full, $J = L + S = 4$.

Solution for 3.2(c)

$$g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} = 1 + \frac{20 + 6 - 6}{40} = 1.5.$$

Note that, since $S = 2$ and $L = 2$, the g value is exactly halfway between that for the $S = 0$ case ($g = 1$) and the spin-only case ($g = 2$).

Solution for 3.2(d)

The total magnetic moment $M = g\sqrt{J(J+1)}\mu_{\mathrm{B}} = 1.5 \times \sqrt{4 \times 5} = 6.7\mu_{\mathrm{B}}$. Since $J = 4, M_J = -4, -3, -2, -1, 0, 1, 2, 3,$ or 4. Therefore the components of the magnetic moment along the field direction, $-gM_J\mu_{\mathrm{B}}$, can take the values $6\mu_{\mathrm{B}}$,

$$4.5\mu_{\mathrm{B}}, 3\mu_{\mathrm{B}}, 1.5\mu_{\mathrm{B}}, 0, -1.5\mu_{\mathrm{B}}, -3\mu_{\mathrm{B}}, -4.5\mu_{\mathrm{B}}, -6\mu_{\mathrm{B}}.$$

In Solution 1.3(b) we calculated the magnetic moment of a "classical" orbiting electron and obtained a result of $1\mu_{\mathrm{B}}$. This is the same order of magnitude as the results obtained here.

Solution for 3.2(e)

If L were equal to zero, then $J = S = 2$ and $g = 2$. So

$$M = 2\sqrt{6}\mu_{\mathrm{B}} = 4.9\mu_{\mathrm{B}}.$$

This is in good agreement with the measured value of $5.4\mu_{\mathrm{B}}$, whereas the moment we calculated using the total angular momentum ($6.7\mu_{\mathrm{B}}$) does not agree well with the experimental value.

This is a manifestation of a phenomenon known as quenching of the orbital angular momentum, which we discuss in Section 5.3.

(??? не знаю, что такое quenching вообще??? ну и все, внезапно с экспериментом не согласуется, что делать???? вообще к такому не готов.)

Solution 1

Если пренебречь различием между центром тяжести молекулы и центром тяжести ядер и считать, что центр тяжести закреплен в начале координат, то уравнение Шредингера для двухатомной молекулы будет иметь следующий вид:

$$\left\{ -\frac{\hbar^2}{2m} \sum_i \left(\frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} \right) - \right.$$
$$- \frac{\hbar^2}{2M_p^2} \left[\frac{\partial}{\partial \rho} \left(p^2 \frac{\partial}{\partial p} \right) + \frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \rho^2} \right] +$$
$$\left. + V\left(x_i, y_i, z_i; \rho, \theta, \varphi\right) \right\} \psi\left(...x_i, y_i, z_i, ...p, \theta, \varphi\right) = E\psi.$$

Здесь $x_i, y_i, z_i \longrightarrow$ координаты i-го электрона относительно неподвижной системы отсчета, углы θ, φ определяют положение в пространстве прямой, соединяющей ядра, ? - расстояние между ядрами, а M - приведенная масса двух ядер. Недостаток этого уравнения заключается в том, что в потенциальную энергию V электростатического взаимодействия входят углы θ и φ. Для того чтобы придать уравнению Шредингера более удобную форму, введем новую систему координат ξ, τ, вращающуюся вместе с ядрами. Ось: направим вдоль прямой, соединяющей ядра, а ось ξ расположим в плоскости xy. Положительное направление оси (?) выберем таким образом, чтобы оси z, ζ, ξ составляли право- винтовую систему. Соотношения между старыми и новыми координатами имеют следующий вид:

$$\xi_i = -x_i \sin\varphi + y_i \cos\varphi,$$
$$\eta_i = -x_i \cos\theta \cos\varphi - y_i \cos\theta \sin\varphi + z_i \sin\theta,$$
$$\zeta_i = x_i \sin\theta \cos\varphi + y_i \sin\theta \sin\varphi + z_i \cos\theta.$$

Различая дифференцирование при постоянных x_i, y_i, z_i от дифференцирования при постоянных ξ_i, η_i, ζ_i штрихом при ∂ находим:

$$\frac{\partial'}{\partial\theta} = \frac{\partial}{\partial\bar{\theta}} + \sum_i \left(\zeta_i \frac{\partial}{\partial r_{ii}} - \eta_i \frac{\partial}{\partial \vartheta_i} \right)$$
$$\frac{\partial'}{\partial\varphi} = \frac{\partial}{\partial\varphi} - \sum_i \left\{ \sin\theta \left(\xi_i \frac{\partial}{\partial \xi_i} - \xi_i \frac{\partial}{\partial \xi_i} \right) + \cos\theta \left(\xi_i \frac{\partial}{\partial \eta_i} \gamma_i \frac{\partial}{\partial \xi_i} \right) \right\}.$$

Легко видеть, что

$$\sum_i \left(\frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} \right) = \sum_i^1 \left(\frac{\partial^2}{\partial \xi_i^2} + \frac{\partial^2}{\partial \eta_i^2} + \frac{\partial^2}{\partial \xi_i^2} \right)$$

Потенциальная энергия в новой системе координат будет иметь вид

$$V = \frac{Z_1 Z_2 e^2}{?} + \sum_{i>k} \frac{e^2}{r_{ik}^*} - \sum_{k=1}^{n} \frac{Z_1 e^2}{r_{1k}^*} - \sum_{k=1}^{n} \frac{Z_2 e^2}{r_{2k}^*},$$

где

$$r_{ik}^* = \sqrt{(\xi_i - \xi_i)^2 + (\eta_i - \eta_i)^2 + (_{-i} - _{\ni h})^2}$$

расстояние между i-ым и k-ым электронами в новых координатах:

$$r_{1k}^* = \sqrt{\xi_k^2 + \eta_i^2 + \left(\zeta_k + p \frac{M_2}{M_1 + M_2} \right)^2}$$

расстояние от k-го электрона до первого ядра и

$$r_{2k}^* = \sqrt{\xi_k^2 + r_{ik}^2 + \left(\zeta_k - \frac{\rho M_1}{M_1 + M_2} \right)^2}$$

расстояние между k-м электроном и вторым ядром. Таким образом в новых координатах потенциальная энергия не зависит от углов θ и о. С учетом всех приведенных соотношений уравнение Шредингера примет следующий вид:

$$\left\{ -\frac{hi}{2m} \sum_i \left(\frac{\partial^3}{\partial \epsilon_i^2} + \frac{\partial^3}{\partial \eta_i^2} + \frac{\partial^2}{\partial \varphi_i^2} \right) ... \right.$$

$$-\frac{l^2}{2M} \frac{1}{r^2} \left[\frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \operatorname{ctg} \theta \left(\frac{\partial}{\partial \theta} - i \grave{L}_\xi \right) + \right.$$

$$\left. + \left(\frac{\partial}{\partial \theta} - i \hat{L}_\xi \right)^2 + \frac{1}{\sin^2 \theta} \left(\frac{\partial}{\partial p} - i \sin \theta \hat{L}_{\eta_p} - i \cos \theta \hat{L}_\Gamma \right)^2 \right] +$$

$$\left. + V \left(\xi_i, \eta_i, i_i^i; p \right) - E \right\} \sim (\xi_i, \eta_i, \vartheta_i; p, 0, \varphi) = 0.$$

Здесь $\hat{L}_\xi, \hat{L}_{\mathrm{r_i}}$ и $\hat{L}_v$ представляют измеренные в единицах $\hbar$ операторы компонент орбитального момента электронов в системе координат $\xi, \eta, \not\vdash$.

1+1

Обознатим спиновую переменную i-го электрона относительно неподвижного пространства через s_i', а относительно подвижного через s_i. Функции $\psi(...s_i...)$ со спинами, отнесенными к координатной системе $\xi\vartheta^\circ$, связаны с функциями (?????) $(... \ s_i'..)$ со спинами, отнесенными к координатной системе xyz линейным преобразованием

$\psi(...s_i...) =$

$$= \sum_{s_1', s_i' ...} S(s_1, ..., s_i, ..., s_1', ..., s_i', ...) \psi_i(...s_i'...) =$$

$$= \hat{S}_\top'(..., s_i'...),$$

где

$S(s_1, s_2, ..., s_i, ..., s_1', ..., s_i', ...) =$

причем

$= S(s_1; s_1') S(s_2; s_2') ...S(s_i; s_i') ...$

$$S\left(\frac{1}{2}; \frac{1}{2} \right) = \cos \frac{\theta}{2} e^{\frac{i}{2}(\varphi + \frac{\pi}{2})}.$$

$$S\left(\frac{1}{2}; -\frac{1}{2} \right) = i \sin \frac{\theta}{2} e^{-\frac{i}{2}(\varphi + \frac{\pi}{2})},$$

$$S\left(-\frac{1}{2}; \frac{1}{2} \right) = i \sin \frac{\theta}{2} e^{\frac{i}{2}(\varphi + \frac{\pi}{2})},$$

$$S\left(-\frac{1}{2}; -\frac{1}{2} \right) = \cos \frac{0}{2} e^{-\frac{i}{2}(\varphi + \frac{\pi}{2})}$$

Мскомое уравнение Шредингера будет иметь вид

$$\left[\grave{S}\hat{H}\hat{S}^{-1} - E\right] \circlearrowleft \left(...\xi_i, r_{ii}, \overleftarrow{-i}, s_i ...; p, \theta, \varphi\right) = 0,$$

где $\grave{H}$ - оператор Гамильтона, наЙденный при решении предыдущей задачи.

Производя несложные вычисления окончательно, для уравнения Шредингера получаем следующее выражение:

$$\left\{-\frac{\hbar^2}{2m}\sum\left(\frac{\partial^2}{\partial\xi_i^2}+\frac{\partial^2}{\partial r_i^2}+\frac{\partial^2}{\partial\epsilon_i^2}\right)-\right.$$
$$-\frac{\hbar^2}{2M}\frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\operatorname{ctg}\theta\left(\frac{\partial}{\partial\theta}-i\grave{M}_\xi\right)+\left(\frac{\partial}{\partial\theta}-iM_\xi\right)^2+\right.$$
$$\left.+\frac{1}{\sin^3\theta}\left(\frac{\partial}{\partial\varphi}-i\sin\theta\grave{M}_r-i\cos\theta\grave{M}_r\right)^2\right]+$$
$$\left.+V-E\right\}\uplus\left(...\xi_i,\eta_i,\overset{\varphi}{-i},s_i...;p,\theta,\varphi\right)=0.$$

Здесь $\hat{M}_\xi, \hat{M}_\eta, \grave{M}$ представляют, в отличие от предыдущей задачи, операторы компонент полного момента электронов (орбитального и спинового).

1+2

Предположим, что задача с неподвижными центрами решена, т. е. известны электронные термы $E^{9.\pi}(\rho)$ и волновая функция $\Phi_{\text{элт}}$ Для определенности рассмотрим тип связи a; пусть в состоянии, описываемом волновой функцией $\Phi_{\text{эл},}$, проекция полного момента (орбитального и спинового) на ось молекулы равна Q. Умножим уравнение Шредингера

$$\hat{H}\Phi_{9,\text{I}}\left(\xi_i,\eta_i,\vartheta_i;\sigma_i;p\right)f(\rho)\Theta((),\varphi)=$$
$$=E\Phi_{9M}\left(\xi_i,\eta_i,\zeta_i;\sigma_i;\rho\right)f(\rho)\theta(\sigma,\varphi)$$

слева на Φ_π^* и проинтегрируем по координатам задачи с неподвижными центрами и просуммируем по σ_i. Замечая, что

$$\int\Phi_{9\pi}^*\hat{M}_\xi\Phi_\pi d\tau=\int\Phi_{9.\text{I}}^*\hat{M}_\eta\Phi_\pi d\tau=0,$$

имеем:

$$\left[B\frac{\partial}{\partial\rho}\left(\rho^2\frac{\partial}{\partial^\rho}\right)-E^{9.T}(\rho)-U(\rho)-E^{\mathbb{B}p}+E\right]f(\rho)=0,$$
$$B\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\left(\frac{\partial}{\partial\varphi}-iQ\cos\theta\right)^2\right]\Theta(\theta,\varphi)+$$
$$+E^{\text{Bp}}\theta(\theta,\varphi)=0.$$

В поспедних двух уравнениях введены спедующие сокращенные обозначения:

$$U(p)=\frac{1}{M}\int\Phi_{\theta\pi}^*\left\{\frac{1}{\rho^3}\left(\hat{M}_5^2+\hat{M}_\eta^2\right)-\frac{\partial^2}{\partial\rho^2}\right\}\Phi_{\partial x}d\tau,$$
$$B=\frac{\hbar^2}{2M}\frac{1}{p^2}.$$

Величина B называется ротационной постоянной.

1+3

Молекула N_2 (атомы в состоянии ^4S): $^1\Sigma_g^+$, $^3\square_u^+$, $^5\Sigma_g^+$, $^7\Sigma_u^+$

Молекула Br_2 (атомы в состоянии ^2P):

$$2^1\Sigma_g^+,\ ^1\Sigma_u-{}^1\Pi_g,{}^1\Pi_u,{}^1\Delta_g;$$
$$2^3\Sigma_u^+,\ ^3\Sigma_g^-,{}^3\Pi_g,{}^3\Pi_u,{}^1\Delta_u.$$

Молекула LiH (атом Li в состоянии ^2S_y, атом H в состоянии $^2S_\S$) : $^1\Sigma^+, 3\Sigma^+$.

Молекула HBr (атом Br в состоянии ${}^2P_u$): $\left[{}^{1\Sigma^+}, {}^3\Sigma^+, Ш^1, 3\right]$. Молекула CN (атом C в сосгоніини ${}^3P_g$, атом N в состоянии ${}^4S_u$) : $2\Sigma^+, 4\Sigma^+, 6\Sigma+, 2\Pi$, ${}^4\Pi, 6\Pi$.

(Число, стоящее перед символом терма, указывает количество термов.)

1+4

Атом гелия в основном состоянии характеризуется тем, что оба его электрона находятся на наиболее низком уровне (парагелий). Полная собственная функция основного состояния атома гелия может быть приближенно представлена в виде

$$\frac{1}{\sqrt{2}}\bigcup_a(1)\bigcup_a(2)\left\{\eta_+\left(\sigma_1\right)\eta_-\left(\sigma_2\right)-\eta_!\left(\sigma_2\right)\eta_-\left(\sigma_1\right)\right\}$$

где $\dot{\psi}_a$ - есть водородная функция.

Атом водорода имеет собственную функцию

$$\bigcup_b(3)\eta_+\left(\sigma_3\right)\ \text{ или }\ \bigcup_0(3)\eta_-\left(\sigma_3\right).$$

Если оба атома находятся на большом расстоянии друг от друга, то волновая функция системы напишется в виде произведения

$\frac{1}{\sqrt{2}}\psi_a(1)\psi_a(2)\bigcup_b(3)\left\{r_1\left(\sigma_1\right)\eta_-\left(\sigma_2\right)-r_{1+}\left(\sigma_2\right)\eta_1\left(\sigma_1\right)\eta_{i!}\left(\sigma_3\right),\right.$ С учетом обмена электронами собственная функция системы должна быть антисимметричной относительно перестановки всех электронов. Существует только одна антисимметричная собственная функция, которая и является собственной функцией нашей системы в нулевом приближении

$$\begin{aligned}\Psi=\frac{1}{\sqrt{6(1-S)}}\{&\psi_a(1)\psi_a(2)\psi_b(3)\left[\eta_+(1)\eta_-(2)-\right.\\&\left.-\eta_+(2)\eta_-(1)\right]\eta_+(3)+\\&+\psi_a(3)\psi_a(1)\psi_b(2)\left[\eta_{i_+}(3)\eta_-(1)-\eta_+(1)\eta_-(3)\right]\eta_+(2)+\\&+\psi_a(2)\psi_a(3)\psi_b(1)\left[\eta_+(2)\eta_-(3)-\eta_+(3)\eta_-(2)\right]\eta_{+-}(1)\}.\end{aligned}$$

В выражении (1) $\frac{1}{\sqrt{6(1-S)}}$ ес ←ь нормировочный множитель, а

$$\begin{aligned}S&=\int\psi_a(1)\psi_a(2)\psi_b(3)\psi_a(2)\dot{\ddots}_a(3)\psi_b(1)d\tau_1d\tau_2d\tau_3=\\&=\int\psi_a(1)\psi_a(2)\psi_b(3)\psi_a(1)\psi_a(3)\psi_b(2)d\tau_1d\tau_2d\tau_3=\\&=\int\psi_a(1)\psi_a(3)\psi_b(2)\psi_a(2)\psi_a(3)\psi_b(1)d\tau_1d\tau_2d\tau_3.\end{aligned}$$

Применяя обычную тсорию возмущения, имеем:

$$\varepsilon=\sum_\sigma\int\Psi\hat{H}\Psi d\tau,$$

гце Ψ - собственная функция в нулевом приближении, $\hat{H}$ - энергия возмущения, суммирование производится по спиновым переменным. Нужно иметь ввнду, что $\grave{H}$ имеет различное выражение для разных составных частей Ч', а именно: для $\psi_a(1)\lhd_a(2)\psi_b(3)$ энергия возмущения равна

$$\hat{H}=e^2\left(\frac{2}{R}-\frac{1}{r_{a3}}-\frac{1}{r_{b1}}-\frac{1}{r_{l2}}+\frac{1}{r_{13}}+\frac{1}{r_{23}}\right),$$

а для $\vartheta_a(1)\psi_a(3)\uplus_b(2)$

$$\hat{H}=e^2\left(\frac{2}{R}-\frac{1}{r_{c2}}-\frac{1}{r_{l1}}-\frac{1}{r_{b3}}+\frac{1}{r_{12}}+\frac{1}{r_{32}}\right).$$

Принимая во внимание то, что интегралы, отличающиеся только нумерацией электронов, идентичны, имеем:

$$\varepsilon=\frac{K-A}{1-S},$$

где

$$K = e^{-2} \int \left(\frac{2}{R} + \frac{1}{r_{13}} + \frac{1}{r_{33}} - \frac{1}{r_{a3}} - \frac{1}{r_{b1}} - \frac{1}{r_{b2}} \right) \times$$
$$X\psi_a^2(1)\psi_a^2(2)\psi_b^2(3)d\tau_1 d\tau_2 d\tau_3$$
$$A = e^2 \int \left(\frac{2}{R} + \frac{1}{r_{13}} + \frac{1}{r_{23}} - \frac{1}{r_{a3}} - \frac{1}{r_{b1}} - \frac{1}{r_{b2}} \right) \times$$
$$X\psi_a\ (1)\ \psi_a(2)\uplus_b(3)\psi_a(1)\psi_a(3)\dot{\psi}_b(2)d\tau_1 d\tau_2 d\tau_3.$$

Нтегралы K, A, S в общем имеют одинаковый характер с соответствующими интегралами проблемы молекулы водорода. Вычисление интегралов показывает, что формула (2) соответствует кривой отталкивания. Это справедливо не только для атома ге.ия, но и для всех благородных газов.

1+5

После отделения движения центра инерции для волновой функции относительного движения ядер получим следующее уравнение:

$$\Delta\psi + \frac{2\mu}{h^2}\left[E + 2D\left(\frac{1}{\rho} - \frac{1}{2p^2}\right)\right]\psi = 0.$$

Разделяя переменные в сферических координатах и полагая

$$\psi = \frac{\chi(\rho)}{\rho} Y_{KM}(\theta, \varphi),$$

находим для γ дифференциальное уравнение:

$$\frac{d^2\gamma_0}{dp^2} + \left[-\lambda^2 + \frac{2\gamma^2}{p} - \frac{\gamma^2 + K(K+1)}{p^2}\right]\chi = 0,$$
$$\lambda = \sqrt{\frac{2\mu a^2 E}{h^2}}, \gamma^2 = \frac{2\mu a^2}{h^3} D.$$

Замена переменных $\chi(p) = p^s e^{-\lambda\rho} u(p)$, где $s = \frac{1}{2} + \ +\sqrt{\gamma^2 + \left(K + \frac{1}{2}\right)^2}$, приводит к гипергеометрическому уравнению

$$\rho u'' + (2s - 2\lambda\rho)u' + \left(-2s\grave{\lambda} + 2\gamma^2\right)u = 0.$$

Решение этого уравнения, конечное при $\rho = 0$, имеет следующий вид:

$$u = cF\left(s - \frac{\gamma^2}{\lambda}, 2s, 2\lambda, p\right).$$

В состояниях дискретного спектра волновая функция χ должна стремиться к нулю при $r \to \infty$. Для этого необходимо, чтобы выражение для u сводилось к полиномам:

$$s - \frac{\gamma^2}{\lambda} = -v,$$

где $\mathfrak{v}$-целое неотрицательное число. Из этого условия получаем энергетические уровни

$$E_{vK} = -\frac{\hbar^2}{2\mu \cdot a^2} \frac{r^4}{\left[v + \frac{1}{2} + \sqrt{\gamma^2 + \left(K + \frac{1}{2}\right)^2}\right]^2}.$$

Безразмерный параметр γ^2 пропорционален приведенной массе ядер μ, так что $\gamma^2 \gg 1$. Если v и K не очен велики

$$\boldsymbol{v} \ll \gamma, \quad K \ll \gamma,$$

выражение $E_{v\ \mathrm{E}}$ принимает следующий вид:

$$E_r K = -D + h\omega_0\left(v + \frac{1}{2}\right) +$$
$$+ \frac{h^2}{2\mu \cdot a^2}\left(K + \frac{1}{2}\right)^2 - \frac{3h^2}{2\mu \cdot a^2}\left(v + \frac{1}{2}\right)^2 - \frac{3h^3\left(K + \frac{1}{2}\right)\left(v + \frac{1}{2}\right)}{2\mu^2 a^4 \omega_0},$$

$$\omega_0 = \sqrt{\frac{2D}{\mu a^2}}.$$

Энергия диссоциации приближенно равна

$$E_0 = D - \frac{\hbar\omega_0}{2}.$$

Второй и третий члены в выражении для $E_{\mathrm{I}mathZZ}$ дают энергию колебательного и вращательного движения. Четвертый член учитывает ангармоничность колебаний и, наконец, пятый член дает поправку к энергии за счет взаимодействия между вращением и колебанием ядер.

Поскольку D есть величина порядка единицы в атомных единицах ($e = m = \hbar = 1$), из полученного выражения следует, что

$$D : \hbar\omega_0 : \frac{h^2}{2\mu, a^2} \sim 1 : \sqrt{\frac{n}{\mu}} : \frac{m}{\mu},$$

где m - масса электрона. Отсюда видно, что разность энергий между двумя квантовыми состояниями с различным движением электронов (величина порядка D) велика по сравнению с разностью энергий различных колебательных состояний, которая в свою очередь велика в сравнении с расстоянием между вращательными уровнями.

1+6

Находим минимум эффективного потенциала

$$W = -2D\left(\frac{1}{\rho} - \frac{1}{2\rho^2}\right) + \frac{A^2}{\rho^2}, \text{ где } \quad A^2 = \frac{\hbar^2 K(K+1)}{2\mu a^2},$$

из условия равенства нулю его производнон:

$$W' = -2D\left(-\frac{1}{\rho_0^2} + \frac{1}{\rho_0^3}\right) - \frac{2A^2}{\rho_0^3} = 0,$$

откуда получаем:

$$P_0 = 1 + \frac{A^2}{D}.$$

Разложим теперь эффективный потенциал вблизи найденного положения равновесия:

$$W(p) \approx -2D\left(\frac{1}{\rho_0} - \frac{1}{p_0^2}\right) + \frac{A^2}{p_0^2} + \frac{D + A^2}{\rho_0^4}\left(p - p_0\right)^2,$$

удерживая здесь члены порядка A^2, получаем:

$$W(p) \approx -D + A^2 + \left(D - 3A^2\right)\left(p - p_0\right)^2.$$

Подставим это выражение в уравнение для %

$$\frac{d^2\chi}{dp^2} + \frac{2\mu a^2}{\hbar^2}\left[E + D - A^2 - \left(D - 3A^2\right)\left(p - p_0\right)^2\right]\chi = 0.$$

Отсюда находим энергетические уровни:

$$E_{vK} = -D + A^2 + \hbar\omega\left(v + \frac{1}{2}\right).$$

Здесь в том же приближении

$$\omega = \omega_0\left(1 - \frac{3}{2}\frac{A^2}{D}\right), \quad \omega_0 = \sqrt{\frac{2\bar{D}}{\mu a^2}}.$$

Окончательно для энергии $E_{\mathrm{I}math\boldsymbol{\kappa}}$ имеем:
$E_{vK} = -D + h\omega_0\left(v + \frac{1}{2}\right) +$

$$+\frac{\hbar^2 K(K+1)}{2\mu a^2} - \frac{3}{2}\frac{\hbar K(K+1)\left(v + \frac{1}{2}\right)}{\mu^2 a^4 \omega_0}.$$

Вследствие того, что при этом вычислении не учитывался эффект ангармоничности, здесь отсутствует член $-\frac{3h^2}{2\mu a^2}\left(v + \frac{1}{2}\right)^2$, полученный при решении предыдущей задачи.

1+7

В инфракрасной полосе мы имеем дело с переходами в основном электронном состоянии, при которых изменяются колебательные и вращательные квантовые числа. Для частоты перехода между двумя состояниями $\tau', J' \to v'', J''$ имеем:

$$\omega = \omega_0 (v' - v'') + \frac{\hbar}{2\mu a^3} \left[J^2 + J' - J'' - J'' \right].$$

Из правил отбора для J следует $J'' = J' \pm 1$. При этом получается совокупность частот

$$\omega = \omega_0 (v' - v'') - \frac{\hbar}{2ua^2} 2 (J' + 1) \quad \left(\begin{array}{l} J'' = J' + 1, \\ J' = 0, 1, 2, \ldots \end{array} \right)$$

и

$$\omega = \omega_0 (v' - v'') + \frac{\hbar}{2\mu a^2} 2J' \quad \left(\begin{array}{l} J'' = J' - 1, \\ J' = 1, 2, \ldots \end{array} \right)$$

Отметим, что эти два' ряда частот в молекулярной спектроскопии называются соответственно P и R ветвью.

Из полученных выражений видно, что разность частот двух соседних линий при фиксированных v' и v'' равна В $C \cdot M^{-1}$

$$\Delta v = \frac{\Delta \omega}{2\pi c} = \frac{\hbar}{2\pi c \mu a^2}.$$

Момент инерции молекулы HCl^{35}

$$I = \mu a^2 = \frac{\hbar}{2\pi c \Delta v} = 2,65 \cdot 10^{-40} 2 \cdot c\mu^2.$$

Используя значение приведенной массы

$$\mu = M_{\mathrm{HI}} \frac{1 \cdot 35}{1 + 35} = 0,972 M_{\mathrm{H}} = 1,61 \cdot 10^{-24} 2,$$

находим расстояние между ядрами в HCl:

$$a = \sqrt{\frac{I}{\mu}} = 1,29 \cdot 10^{-8} \text{см}.$$

Равновесные расстояния a в молекулах DCl и HCl одинаковы, поскольку форма потенциальных кривых определяется состоянием электронов. Отсiода следует, что

$$\frac{\Delta v_{\mathrm{DCI}}}{\Delta v_{\mathrm{HCI}}} = \frac{\mu_{\mathrm{HCI}}}{\mu_{\mathrm{DCI}}}; \quad \Delta v_{\mathrm{DCI}} = 10,7 c\mu^{-1}.$$

1+8

Расстояние между двумя первыми врацательными уровнями

$$\Delta v_{\mathrm{Bp}} = \frac{\hbar}{2\pi c I} = 41,5 \text{см}^{-1}.$$

Отсюда находим:

$$\frac{\Delta v_{\mathrm{Bp}}}{\Delta v_{\mathrm{F0I}}} = 0,0104.$$

1+9

Энергия диссоциации молекулы D_2 равна 4,54 эв.

Переходя К новой переменной $\xi = \frac{r-a}{a}$, запишем уравнение для радиальной функции $\frac{\chi}{r}$:

$$\frac{d^2\chi}{d\xi^3} + \frac{2i^3 a^2}{\hbar^2} (E - V)\% = 0.$$

Полагая $z = \alpha e^{-2\beta \frac{2}{5}}$, получим:

$$\chi'' + \frac{1}{z}\chi' + \left(-\frac{s^2}{z^3} - \frac{1}{4} + \frac{v+s+\frac{1}{2}}{z}\right)\chi = 0$$

где

$$s = \sqrt{\frac{\mu a^2(D-E)}{\beta^2\hbar^2}}, \quad v+s+\frac{1}{2} = \frac{\mu a^2 D}{\alpha\beta^2\hbar^2}, \quad a^2 = \frac{2\mu a^2 D}{\beta^2\hbar^3}.$$

Полученное уравнение заменой $= e^{-\frac{z}{2}} z^s u(z)$ сводится к гигергеометрическому $zu'' + (2s+1-z)u' + nu = 0$, решением которого является вырожденная гипергеометрическая функция $u = F(-v, 2s+1, z)$. Эта функция удовлетворяет условию обращения % в нуль при $r \to +\infty$ при положительных значениях s (дискретный спектр). При $r \to -\infty$ волновая Функция должна обрацаться в нуль. Для выполнения этого условия необходимо, чтобы F сводилось к полиномам, т. е. чтобы v было неотрицательным целым числом. Это условие определяет энергетический спектр

$$E_n = \hbar\omega\left(v+\frac{1}{2}\right) - \frac{\hbar^2\omega^2}{4D}\left(v+\frac{1}{2}\right)^2, \quad \text{где} \quad \omega = 4\beta\sqrt{\frac{D}{2\mu a^2}}.$$

Таким образом, расстояние между колебательными уровнями уменьшается с увеличением квантового числа $\boldsymbol{v}$.

Энергия диссоциации равна

$$E_0 = D - \frac{\hbar\omega}{2} + \frac{\hbar^2\omega^2}{16D}.$$

1+12

В качестве параметров, характеризующих вращение, возьмем углы Энлера $(\theta, \bigcup, \varphi)$. В этом случае координаты точки x, y, z в неподвижной системе связаны с координатами ξ, η, ζ в подвижноћ системе отсчета следующим образом: $x = \xi(\cos\psi\cos\varphi - \sin\psi\sin\varphi\cos\theta) -$

$$\left.\begin{array}{c} -\eta(\cos\psi\sin\varphi + \sin\psi\cos\varphi\cos\theta) + \zeta\sin\psi\sin\theta, \\ y = \xi(\sin\psi\cos\varphi + \cos\psi\sin\varphi\cos\theta) + \\ +\eta(-\sin\psi\sin\varphi + \cos\psi\cos\varphi\cos\theta) - \gamma\cos\psi\sin\theta, \\ z = \xi\sin\varphi\sin\theta + \eta\cos\varphi\sin\theta + \zeta\cos\theta. \end{array}\right\}$$

Для того чтобы найти вид операторов $\hat{J}_\xi, \hat{J}_\eta, \hat{J}_\zeta$, воспольэуемся тем соображением, что оператор $\hat{J}_\xi$ есть $\hat{J}_\xi = -i\frac{\partial}{\partial\alpha}$, где x угол, отсчитываемыи в плоскости, перпендикулярноћи оси ξ. Так как вследствие поворота системы координат ξ, η, ζ относительно, например, оси ξ на бесконечно малый угол $d\alpha$, значения углов изменятся, то мы можем написать, что $\hat{J}_\xi$, измеренный в единицах $\hbar$, равен

$$\hat{J}_\xi = -i\left(\frac{\partial\theta}{\partial\alpha}\frac{\partial}{\partial\theta} + \frac{\partial\varphi}{\partial\alpha}\frac{\partial}{\partial\varphi} + \frac{\partial\psi}{\partial\alpha}\frac{\partial}{\partial\psi}\right).$$

При бесконечно малом повороте относительно оси ξ на угол $d\alpha$ имеем:

$$\left.\begin{array}{ll} \xi & = \xi', \\ \eta & = \eta' - ?' d\alpha, \\ \zeta & = \eta' d\alpha + \zeta' \end{array}\right\}$$

И

$$z = \xi'\sin(\varphi + d\varphi)\sin(\theta + d\theta) + \\ + \eta'\cos(\varphi + d\varphi)\sin(\theta + d\theta) + \zeta'\cos(\theta + d\theta).$$

С другой стороны, подставляя (2) в (1), получаем:
$z = \xi'\sin\varphi\sin\theta + \eta'(\cos\varphi\sin\theta + \cos\theta d\alpha) +$
$+\zeta'(\cos\theta - \cos\varphi\sin\theta d\alpha)$. Сравнивая (3) и (4), находим:

$$\frac{d\theta}{d\alpha} = \cos\varphi, \quad \frac{d\varphi}{d\alpha} = -\sin\varphi\operatorname{ctg}\theta.$$

Поступая аналогичіо, имеем: $\frac{d\downarrow}{d\alpha} = \frac{\sin\varphi}{\sin\theta}$.

Окончательно для $\hat{J}_\xi$ получаем выражение

$$\hat{J}_\xi = -i\left(\cos\varphi\frac{\partial}{\partial\theta} - \sin\varphi\operatorname{ctg}\theta\frac{\partial}{\partial\varphi} + \frac{\sin\varphi}{\sin\theta}\frac{\partial}{\partial\psi}\right).$$

Таким же образом находятся выражения двух других операгоров

$$\hat{J}_\eta = -i\left(-\sin\varphi\frac{\partial}{\partial\theta} - \cos\varphi\operatorname{ctg}\theta\frac{\partial}{\partial\varphi} + \frac{\cos\varphi}{\sin\theta}\frac{\partial}{\partial\iota}\right),$$
$$\hat{J}_\zeta = -i\frac{\partial}{\partial\varphi}.$$

16.

$$E_J = \frac{h^2}{2A}J(J+1)$$

Каждый уровень вырожден $(2J+1)$ раз по направлениям момента относительно неподвижного пространства и столько же раз по направлениям момента относительно самого тела.

1+16

Так как $\hat{H} = \frac{1}{2A}\hat{J}^2 + \frac{1}{2}\left(\frac{1}{C} - \frac{1}{A}\right)\hat{J}_\zeta^2$, то $E = \frac{1}{2A}J(J+1) + \frac{1}{2}\left(\frac{1}{C} - \frac{1}{A}\right)k^2; J_\zeta = k \quad |k| \leqslant J$.

В этом случае полная кратность вырождения уровня равна $2(2J+1)$. Вырождение по направлениям момента в неподвижном пространстве остается по-прежнему равным $(2J+1)$. 18.

$$-\frac{\hbar^2}{2A}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\left(\frac{\partial^2 u}{\partial\rho^2} + \frac{\partial^2 u}{\partial\psi^2}\right) - \right.$$
$$\left. -2\frac{\cos\theta}{\sin^2\theta}\frac{\partial^2 u}{\partial \Downarrow \partial\varphi}\right\} - \frac{\hbar^2}{2}\left(\frac{1}{C} - \frac{1}{A}\right)\frac{\partial^2 u}{\partial\varphi^2} = Eu.$$

1+18

Поскольку с $\hat{J}^2$ коммутируют операторы $\hat{J}_5 = -i\frac{\partial}{\partial\varphi}$ и $\hat{J}_z = -i\frac{\partial}{\partial}$, то собственную функцию будем искать в виле

$$\Phi_{kJM_J} = \boldsymbol{A}_{kJM_J}(\theta)e^{iM_J\psi}e^{ik\varphi},$$

где M_J, k - проекции момента на неподвижную ось z и подвижную ось ?? соответственно.

Так как & и φ входят в уравнение (14) симметрично, а $|k| \leqslant J$, то $|M_J| \leqslant J$.

Рассмотрим операторы

$$\hat{J}_\xi - i\hat{J}_\eta = -ie^{i\vartheta}\left(\frac{\partial}{\partial\theta} + i\operatorname{ctg}\theta\frac{\partial}{\partial\varphi} - \frac{i}{\sin\theta}\frac{\partial}{\partial\zeta}\right).$$

Легко проверить, что

$$\hat{J}_\xi\left(\hat{J}_\xi - i\hat{J}_\eta\right)\Phi_{kJM_J} = (k+1)\left(\hat{J}_\xi - i\hat{J}_\eta\right)\Phi_{kJM_J},$$

т. е. выражение $\left(\hat{J}_\varepsilon - i\hat{J}_r\right)\Phi_{zJ}M_J$ есть собственная функция, соответствующая значению $(k+1)$ оператора $\hat{j}_\xi$.

Положим $k = J$, тогда имеем:

$$\left(\hat{J}_\xi - i\hat{J}_\eta\right)\Phi_{JJ}M_J \equiv 0.$$

Последнее соотношение можно представить в виде

$$\left(\frac{\partial}{\partial\theta} + i\operatorname{ctg}\theta\frac{\partial}{\partial\rho} - \frac{i}{\sin\theta}\frac{\partial}{\partial\varphi}\right)\Theta_{JJ}M_J(\theta)e^{iU_J\psi}e^{iJ\varphi} \equiv 0.$$

Отсюда найдем обыкновенное дифференциальное уравнение первого порядка для определения Θ_{JJM_J}

$$\frac{d\theta_{JJM_J}}{d\theta} + \frac{M_J - J\cos\theta}{\sin\theta}\theta_{JJM_J} = 0.$$

Общее решение этого уравнения имеет вид

$$\theta^J_{JJM} = c\frac{(\sin\theta)^J}{\left(\operatorname{tg}\frac{\theta}{2}\right)^M}$$

Или

$$\theta(\theta) = c(1-\cos\theta)^{\frac{J-M_J}{2}}(1+\cos\theta)^{\frac{J+\pi N_J}{2}}\cdot\Big)$$

Поскольку функция Θ должна быть конечнойћ, то $|M^J| \leqslant J$.

$$\hat{J}_\xi + i\hat{J}_\eta = -ie^{-i\varphi}\Big(\frac{\partial}{\partial\theta} - i\operatorname{ctg}\theta\frac{\partial}{\partial\varphi} + \frac{i}{\sin\theta}\frac{\partial}{\partial\psi}\Big),$$

Для того чтобы определить функцию Θ_{kJM}, рассмотрим действие на нее оператора $\left(\hat{J}_{\bar{\varepsilon}} + i\hat{J}_{r_1}\right)$. Так как

$$\hat{J}_\xi\left(\hat{J}_\xi + i\hat{J}_\eta\right)\theta_{kJM_J} = (k-1)\left(\hat{J}_\xi + i\hat{J}_\eta\right)\theta_{kJM_J},$$

То

$$\left(\hat{J}_\xi + i\hat{J}_\eta\right)\theta_{kJM_J} = \alpha_k\theta_{k-1JM_J}.$$

Подставляя в (4) явный вид оператора $\left(\hat{J}_\xi + i\hat{J}_\eta\right)$ из (1), приходим к уравнению

$$\frac{d\Theta_{kJM_J}}{d\theta} + \frac{k\cos\theta - M_J}{\sin\theta}(\theta_{kJM_J} = i\alpha_i\Theta_{k-1J}M_J,$$

которое после введения переменнойћ $x = \cos\theta$ принимает вид $\sqrt{1-x^2}\frac{dP_{kJM_J}(x)}{dx} + \frac{M_J - kx}{\sqrt{1-x^2}}P_{kJM_J}(x) = -i\alpha_k P_{k-1JM_J}(x)$, где

$$P_{kJM_J}(x) = \theta_{kJM_J}(\arccos x).$$

Положив

$$P_{\boldsymbol{l}JM_J} = (1-x)^{-\frac{(k-M_J)}{2}}(1+x)^{-\frac{(k+M_JJ)}{2}}\widetilde{}_{kJ}M_J,$$

найдем простое соотношение для опредетения $\boldsymbol{v}_{kJ}\mu_J$

$$\frac{dv_{kJM_J}}{dx} = -i\alpha_k v_{k-1JM}J^\circ$$

Ранее найденные функции $P_{JJ\mu_J}$ (см. (3)), можно переписать в виде (5)

$$P_{JJM_J}(x) = (1-x)^{-\frac{(J-MU_J)}{2}}(1+x)^{-\frac{(J+MJ}{2}}v_{JJM_J},$$

где через блы, мы обозначим выражение

$$v_{JJM_J}(x) = c(1-x)^{J-M_J}(1+x)^{J+M_J}.$$

Из (7) и реккурентного соотношения (6) вытекает, что

$$v_{kJM_J} = c\frac{d^{J-k}}{(dx)^{J-k}}\left\{(1-x)^{J-M_J}(1+x)^{J+M_J}\right\}$$

Следовательно,

$$\Phi_{kJM_J}(\varphi,\psi,\varphi) =$$
$$= ce^{ik\varphi}e^{iM_J\psi}(1-\cos\theta)^{-\frac{k-M_J}{2}}(1-\cos\theta)^{-\frac{k+M_J}{2}}\times$$
$$\chi\left(\frac{d}{d\cos\theta}\right)^{J-R}\left\{(1-\cos\theta)^{J-M_J}(1+\cos\theta)^{J+M}J\right\}$$

при $M_J = 0$ эти обобщенные сферические функции переходят, как и следовало ожидать, в обычные сферические функции и представляют собой волновые функции ротатора:

$$\Phi_{k,J}(\theta,\varphi) = ce^{ik\varphi}\frac{1}{\sin^k\theta}\frac{d^{J-k}}{(d\cos\theta)^{J-k}}\left(\sin^{2J}\theta\right).$$

20.

$$\hat{H}_{kk} = \frac{\hbar^2}{4}\left(\frac{1}{A}+\frac{1}{B}\right)\left\{J(J+1)-k^2\right\} + \frac{\hbar^2k^2}{2c},$$

$\hat{H}_{kk+2} = \grave{H}_{k+2k} =$

$$= \frac{\hbar^2}{8}\left(\frac{1}{A}-\frac{1}{B}\right)\sqrt{(J-k)(J-k-1)(J+k+1)(J+k+2)}.$$

1+20

Для асимметрического волчка вырождение по направлениям момента относительно неподвижного пространства все еще остается. Вырождение относительно квантового числа k полностью снимается, так что данному J соответствует $(2J+1)$ различных уровней. В случае $J=1$ уровни энергии определятся из решения секулярного уравнения вида

$$\begin{vmatrix} H_{11}E & H_{10} & H_{1,-1} \\ H_{10} & H_{00}E & H_{0-1} \\ H_{-11} & H_{-10} & H_{-1,-1}-E \end{vmatrix} = \\ = \begin{vmatrix} H_{11}-E & 0 & H_{1,-1} \\ 0 & H_{00}-E & 0 \\ H_{-1,1} & 0 & H_{-1,-1}-E \end{vmatrix} = 0.$$

Так как $H_{-1,-1}=H_{11}$, то имеем:
откуда

$$(H_{00}-E)\left(H_{11}^2+E^2-2H_{11}E-H_{1,-1}^2\right)=0,$$

$$E_1=\frac{\hbar^2}{2}\left(\frac{1}{A}+\frac{1}{B}\right),\quad E_2=\frac{\hbar^2}{2}\left(\frac{1}{C}+\frac{1}{A}\right),\quad E_3=\frac{h^2}{2}\left(\frac{1}{B}+\frac{1}{C}\right).$$

22.

E		m	
E_1	$\Phi_{k=0,\,m}$	1	$\frac{\sqrt{3}}{4\pi}e^{i\psi}\sin\theta$
		0	$\frac{1}{\pi}\sqrt{\frac{3}{8}}\cos\theta$
		-1	$\frac{\sqrt{3}}{4\pi}e^{-i\psi}\sin\theta$
E_2	$c\,(\Phi_{k=1,\,m}+\Phi_{k=-1,\,m})$	1	$\frac{1}{\pi}\sqrt{\frac{3}{16}}e^{i\psi}(\cos\varphi+i\cos\theta\sin\varphi)$
		0	$\frac{1}{\pi}\sqrt{\frac{3}{8}}\cos\varphi\sin\theta$
		-1	$\frac{1}{\pi}\sqrt{\frac{3}{16}}e^{-i\psi}(\cos\varphi-i\cos\theta\sin\varphi)$
E_3	$c\,(\Phi_{k=1,\,m}-\Phi_{k=-1,\,m})$	1	$\frac{1}{\pi}\sqrt{\frac{3}{16}}e^{i\psi}(\cos\theta\cos\varphi+i\sin\varphi)$
		0	$\frac{1}{\pi}\sqrt{\frac{3}{8}}\sin\theta\sin\varphi$
		-1	$\frac{1}{\pi}\sqrt{\frac{3}{16}}e^{-i\psi}(-\cos\theta\cos\varphi+i\sin\varphi)$

1+23

Расщепление терма обусловлено взаимодействием спин - спин. Для определения искомого расщепления необходимо оператор взаимодействия спин - спин $\alpha(\hat{S}n)^2$ усреднить по вращательному состоянию. При данном K квантовое число J принимает значения

$$J=K+1,K,K-1.$$

Отличные от нуля матричные элементы $(n\hat{S})$ имеют вид

$$(n\hat{S})^{K-1}_{K}{}^{J=K}_{J=K}=(n\hat{S})^{K}_{K-1,J=K}=\sqrt{\frac{K+1}{2K+1}},$$
$$(n\hat{S})^{K}_{K-1}{}^{J=K-1}_{J=K-1}=(n\hat{S})^{K-1}_{K}\overline{\frac{K-1}{J=K-1}}.\sqrt{\frac{K-1}{2K-1}}.$$

Пользуясь последними соотношениями, находим искомое расщепление компонент триплета:
$\Delta E_{J=\boldsymbol{K}+1}=\frac{K+2}{2K+3}\alpha,\quad \Delta E_{J=\boldsymbol{K}}=\alpha,\quad \Delta E_{J=K-1}=\frac{K-1}{2K-1}\alpha$

18.1.12 Advanced problems about molecules

1+24

Найдем прежде всего недиагональные элементы оператора w

$$\{w\}^{n\Delta Qv}_{n\Delta\Omega' vJ'}$$

Легко видеть, что отличны от нуля только матричные элементы, соответствующие $Q' = Q \pm 1, J = J'$. Так как

$$\{\hat{M}_\xi\}^{n\Delta\Omega}_{n\Delta\Omega\pm 1} = \mp i \{\hat{M}_\eta\}^{n\Delta\Omega}_{n\Delta\Omega\pm 1},$$

то

$$\{\tau v\}^{n\Delta 2vJ}_{n\Delta Q\pm 1vJ} = \frac{\hbar^2}{M}\left\{\pm\frac{\partial}{\partial\theta} + \frac{i}{\sin\theta}\frac{\partial}{\partial p} + (Q\pm 1)\operatorname{ctg}\theta\right\}^{\Delta 2J}_{\Delta Q\pm 1J} \times \times \left\{\frac{1}{\rho^2}\hat{M}_{\tau_i}\right\}^{n\Delta Qv}_{n\Delta Q\pm 1v}.$$

Для вычисления матричного элемента

$$\left\{\pm\frac{\partial}{\partial\theta} + \frac{i}{\sin\theta}\frac{\partial}{\partial\dot{\varphi}} + (Q\pm 1)\operatorname{ctg}\theta\right\}^{\Delta QJ}_{\Delta Q\pm 1J},$$

заметим, что если в операторе $(J_\xi + iJ_{r_1})$ (см. задачу 13§ 8) положить угол $\varphi = 0$, а $-i\frac{\partial}{\partial\varphi} \to \hat{M}_\zeta$, то

$$(J_\xi \pm iJ_{r_i})_\xi \to 0$$
$$-i\frac{\partial}{\partial\varphi} \to \mp i\left\{\pm\frac{\partial}{\partial\theta} + \frac{i}{\sin\theta}\frac{\partial}{\partial\varphi} + (Q\pm 1)\operatorname{ctg}\theta\right\}.$$

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$$(n\hat{S})^{K+1\ J=K}_{K\ \ J=K} = (n\hat{S})^{K\ \ J=K}_{K+1\ J=K} = \sqrt{\frac{K}{2K+1}},$$

$$(n\hat{S})^{K\ \ J=K+1}_{K+1\ J=K+1} = (n\hat{S})^{K-1\ J=K+1}_{K\ \ J=K+1} = \sqrt{\frac{K+2}{2K+3}},$$

Учитывая последнее соотношение, имеем:

$$\left\{\pm\frac{\partial}{\partial\theta} + \frac{i}{\sin\theta}\frac{\partial}{\partial\dot{\rho}} + (Q\pm 1)\operatorname{ctg}\theta\right\}^{\Lambda QJ}_{\Delta Q\pm 1J} =$$
$$= \pm i\sqrt{(J\mp Q)(J\pm Q+1)}.$$

В случае малых колебаний около положения равновесия матричный элемент

$$\left\{\frac{1}{p^2}\hat{M}_\eta\right\}^{n\Delta Qv}_{n\Delta Q\pm 1v}$$

приближенно можно положить равным

$$\frac{1}{p_0^2}\left\{\hat{M}_n\right\}^{n\Lambda\Omega}_{n\Delta\Omega\pm 1},$$

где p_0 - расстояния между ядрами в положении равновесия. Так как
$\left\{\hat{L}_\eta + \hat{S}_n\right\}^{n\Delta\Omega}_{n\Delta Q\pm t} = \left\{\hat{S}_\eta\right\}^{n\Delta Q}_{n\Delta Q\pm 1} = \pm\frac{i}{2}\sqrt{S(S+1) - \sum(\sum\pm 1)}$
то окончательно имеем:

$$\{w^{n\Delta 8}_{n\Delta\varepsilon\pm 1vJ} =$$
$$= B_0\sqrt{S(S+1) - \Sigma(\Sigma\pm 1)}\sqrt{J(J+1) - (\Lambda+\Sigma)(\Lambda+2-1-1.}$$

Здесь $B_0 = \frac{\hbar^2}{2M\rho_0^2}$ представляет собой значение ротационноĥi постоянной для состояния равновесия, отвечающего некоторому $p = P_0$.

В общем случае дублетное расцепление может быть равно по порядку вычисленным маятрнчным элементам. Поэтому д.яя расчета смещения уровней дублетного терма применим теорию возмущения в несколько измененном виде. В качестве исходного нулевого приб.иижения возьмем вместо функций

$$\psi_{n\Delta A+1} \le vJ, \quad i_{n\Delta\Delta-1'_i vJ}$$

их линейную комбинацию

$$\dot{\psi} = c_1\psi i\Delta\Delta\Delta + 1, vJ + c_2\psi_{n\Delta\Delta-1/2v}J.$$

Подставляя это выражение в возмущенное уравнение и поступая стандартным образом, находим секулярное уравнение

$$\begin{vmatrix} E^{(0)}_{n\Delta\Delta+1/2vJ} - E & w^{n\Delta\Delta+1/2vJ}_{n\Delta\Delta-1/2vJ} \\ w^{n\Delta\Delta-1/2vJ}_{n\Delta\Delta+1/2vJ} & E^{(0)}_{n\Delta\Delta-1/2vJ} - E \end{vmatrix} = 0.$$

Из решения секулярного уравнения следует, что

$$E = \frac{1}{2}E^{(0)} \pm \frac{1}{2}\sqrt{\Delta E^{(0)} + 4B_0^2\left\{\left(J+\frac{1}{2}\right)^2 - \Lambda^2\right\}}$$

где

$$E^{(0)} = E^{(0)}_{n\Delta\Delta+1_2v} + E^{(0)}_{n\Delta\Delta-1:vJ}$$
$$\Delta E^{(0)} = E^{(0)}_{n\Delta\Delta\div 1_2vJ} - E^{(0)}_{n\Delta A-1\vdots\Delta vJ}$$

В случае связи a, когда мультиплетное расщепление велико по сравнению с вращением, из соотношения (1) приближенио следует, что

$$E_1 = E^{(0)}_{n\Delta\Delta+1'_2vvJ} + \frac{B_0^2\left\{\left(J+\frac{1}{2}\right)^2 - \Lambda^2\right\}}{\Delta E^{(0)}},$$
$$E_2 = E^{(0)}_{n\Delta\Delta-1!_2vJ} - \frac{B_0^2\left\{\left(J+\frac{1}{2}\right)^2 - \Lambda^2\right\}}{\Delta E^{(0)}}.$$

В случае связи b из (1) получаем:
$E_{1,2} = \frac{1}{2}E^{(0)} \pm B_0\left\{\left(J+\frac{1}{2}\right)^2 - \Lambda^2\right\} \pm \frac{\Delta E^{(0)}}{8B_0\left\{\left(J+\frac{1}{2}\right)^2 - \Lambda^2\right\}}$

1+25

$K = 0, 2, 4, ...$, если суммарный спин $S = 2$ или $S = 0$, $K = 1, 3, 5, ...$, если суммарный спин $S = 1$.
Магнитный момент молекулы равен $\frac{e\hbar}{2mc}(\Lambda + 2\Sigma)n$, где $\boldsymbol{n}$ - единичный вектор, направленный по оси молекулы.
Длля определения энергии расщепления необходимо усреднить величину

$$-\frac{e\hbar}{2mc}(1 + 2\Sigma)ngl$$

по вращательному состоянию, т. е. определить матричные элементы

$$(n)^{JM_j}_{JNI_j}$$

Так как $\hat{J}$ есть единственный сохраняющийся вектор, то очевидно, что матричные элементы вектора $\boldsymbol{n}$ будут пропорциональны матричным элементам вектора $\hat{J}$, т. е.

$$(\boldsymbol{n})^{JMM'_j}_{JM_j} \sim (J_J)^{JM'_j}_{JM_j}.$$

Рассматривая $\boldsymbol{n}$ как оператор, имеем:

$$\hat{\boldsymbol{n}} = \text{ const } \hat{J}.$$

Для определения константы умножим последнее выражение слева и справа на $\hat{\boldsymbol{J}}$. Так как собственные значения $\hat{\boldsymbol{J}}^2$ равны $J(J+1)$, а $\hat{J}\hat{n}$ равны Q, то имеем:

$$\grave{n} = \frac{\Omega}{J(J+1)}\grave{J}.$$

Таким образом, оператор энергии возмущения равен

$$-\frac{e\hbar}{2mc}(\Lambda + 2\Sigma)\cdot\frac{\varrho}{J(J+1)}\mathscr{J}\hat{J}.$$

Вычисляя диагональные матричные элементы, получаем для энергии расщепления выражение следующего вида:

$$\Delta E_{M_j} = -\frac{e\hbar_{\mathcal{H}}}{2mc}(\Lambda + 2\Sigma)\frac{\Omega}{J(J+1)}M_j.$$

1+27

Оператор возмущения, как легко установить, в данном случае имеет следующий вид:

$$-\frac{eh_l}{2m\bar{c}}\mathscr{H}\left\{\frac{\Lambda^2}{K(K+1)}\dot{K} + 2\dot{S}\right\}.$$

Отсюда следует, что зеемановское расщепление равно $\Delta E_{M_j} = -M_j \frac{e\hbar\%\mathcal{C}}{2mc}\times$
$\times\left\{\Lambda^2\frac{J(J+1)-S(S+1)+K(K+1)}{2K(K+1)J(J+1)} + \frac{J(J+1)+S(S+1)-K(K+1)}{J(J+1)}\right\}$.

1+28

Энергия зеемановского расщепления равна

$$\Delta E_{MK^M}M_{\mathrm{S}} = -\frac{e\hbar}{2mc}\mathscr{K}^{2m}\left[\frac{\Lambda^2}{K(K+1)}M_K + 2M_{\mathrm{S}}\right].$$

1+29

Так как энергия взаимодействия магнитного момента с внешним магнитным полем одного порядка с энергией взаимодействия спин- ось, то их надо рассматривать в теории возмущения одновременно. Оператор возмущения имеет В Нд

$$\hat{V} = An\hat{\mathbf{S}} - \mu_0 \Delta n\mathfrak{H} - 2\mu_0\hat{\mathbf{S}}\mathfrak{H}.$$

В качестве волновых функций нулевого приближения возьмем волновые функцни состояний, в которых имеют определенные значения момент K и проекция K и S на направление магнитного поля. Ось z направим по магнитному полю. Так как проекция полного момента на направлени е магнитного поля сохраняется, то в случае дублетного терма мы должны применить теорию возмущения при наличии двухкратного вырождения. Вычисляя матричные элементы оператора возмущения, имеем:

$$\begin{aligned}
&V^{1/K}_{N_K,-1!2}, {}^{-1!} = -M_K\frac{1}{2K(K+1)}A - M_K\frac{\Lambda^2}{K(K+1)}\mu_0\mathscr{H} + \mu_0\mathscr{H},\\
&V^{U_K-1,!_2}_{N_K} = (M_K-1)\frac{1}{2K(K+1)}A -\\
&-(M_K-1)\frac{\Lambda^2}{K(K+1)}\mu_0\mathscr{F} - \mu_0\mathscr{H}O,\\
&V^{M_K^{-1,2}}_{N_K-1,1_{i,2}} = \frac{1}{2}A\frac{1}{K(K+1)}\sqrt{(K-M+1)(K+M)} =\\
&= \frac{1}{2}A\left\{n_x + in_y\right\}^{N_K}_{N_K K^{-1}},\\
&= \frac{1}{2}A\frac{\Lambda}{K(K+1)}\sqrt{(K-M+1)(K+M)}.
\end{aligned}$$

Составляя и решая секулярное уравнение, получим:

$$E^{(1)}_{1,2} = \frac{\lambda^2}{K(K+1)}\left(M_K - \frac{1}{2}\right)\mu_0 A - \frac{A\Lambda}{4K(K+1)} \pm \frac{1}{2K(K+1)}\times$$
$$\times\sqrt{\left\{A\Lambda\left(M-\frac{1}{2}\right) - \Lambda^2\mu_0\mathscr{H} + 2\mu_0\mathscr{O}(K+1)K\right\}^2 + A^2\Lambda^2\left(K+M_K\right)\left(K-M_K+1\right)}.$$

Рассмотрим предельные случаи.
Если $\mu_0 \nrightarrow \gg A$, то для $E^{(1)}_{1,2}$ получаем выражение

$$E_{1,2}^{(1)} = -\frac{\Lambda^2}{K(K+1)}\left\{M_K - \frac{1}{2} \mp \frac{1}{2}\right\}\mu_0\mathscr{H} \leftarrow \mu_0\mathcal{L}?,$$

согласующееся с формулой, полученной в задаче 29§8.

$$V_{M_K,\,-1/2}^{M_K-1,\,1/2} = \frac{1}{2}A\{n_x - in_y\}_{M_K}^{M_K-1} =$$

При $A \gg \mu_0\mathscr{H}$ получается

$$E_1^{(1)} = \frac{A\Lambda}{2(K+1)} - \left(M_K - \frac{1}{2}\right)\left\{\frac{\Lambda^2}{(K+1)\left(K+\frac{1}{2}\right)} + \frac{1}{K+\frac{1}{2}\}}u_0\mathscr{H},$$

$$E_2^{(1)} = -\frac{A\Lambda}{2K} - \left(M_K - \frac{1}{2}\right)\left\{\frac{\Lambda^2}{K\left(K+\frac{1}{2}\right)} - \frac{1}{K+\frac{1}{2}\}\mu_0\mathcal{H}^\circ}.$$

Вторые члены последних формул, т. е. члены, зависящие линейно от ёf, совпадают с соответствующими выражениями, которые получаются при подстановке в формулу, найденную в задаче 28£8,

$$J = K \pm 1/2, \quad S = 1/2 \text{ и } \quad M_j = M_K - 1/2^\circ$$

1+30

В силу аксиальной симметрии дигольный момент молекулы направлен по прямой, соединяющей ядра, т. е.

$$\boldsymbol{p} = p\boldsymbol{n}.$$

Поступая так же, как и при решении задачи 27$8, находим:

$$\Delta E_{M_j} = \ldots_p\frac{\Omega}{J(J+1)}M_j.$$

32.

$$\Delta E_M = -8pM_j\Lambda\frac{J(J+1) - S(S+1) + K(K+1)}{2K(K+1)\cdot J(J+1)}.$$

1+32

Поправка первого приближения к энергии равна нулю. Как известно, поправка второго приближения к энергии в случае вырождения находится из условия совместности однородных линейных уравнений

$$E_n^{(2)}c_{n\xi}^{(0)} = \sum_j c_{nj}^{(0)}\sum_{ma}\frac{V_{ma}^{n\beta}V_{nj}^{ma}}{E_n^{(0)} - E_{ni}^{(0)}}$$

'В нашем случае из последнего соотношения получаем:

$$E_{lmb}^{(2)} = \frac{p^2g^2A}{h^2}\left\{\frac{l^2 - m^2}{(2l+1)(2l-1)l} - \frac{(l+1) - m^2}{(2l+3)(2l+1)(l+1)}\right\}.$$

Таким образом энергия твердого диполя равна

$$E_{lm} = \frac{\hbar^2}{2A}l(l+1) + E_{l,n}^{(2)}; \quad E_{00} = -\frac{1}{3}\frac{Ap^2g^2}{h^2} \quad (l=0).$$

Этот результат до некоторой степени парадоксален. В самом деле, согласно последнему равенству энергия твердого диполя пропорциональна не &, a&^{2}. Следовательно, твердому диполю формально можно приписать определенную «поляризуемость».

Рассмотрим случай, когда $l = 1$. Уровень, соответствующий значению $m = 0$, обладает в электрическом поле большей энергией, чем вне его, так что соответствующая молекула ведет себя так, как будто она обладает отрицательной поляризуемостью.. - Она ведет себя подобно диамагнитному телу в магнитном поле. Молекула в состоянии $m = \pm 1$

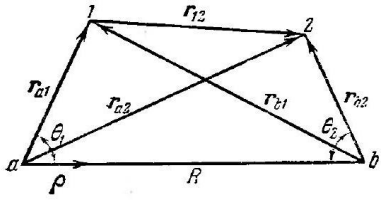

Рис. 31.

ведет себя «нормально». Вырождение в электрическом поле снимается только частично, поскольку энергия зависит только от абсолютного значения проекции момента количества движения.

Отметим, что $\sum_{m=-l}^{m=+l} E_{lm}^{(2)} = 0$.

1+33

При больших значениях R можно пренебречь обменом, т. е. считать, что первый электрон находится при ядре a, а второй электрон - при ядре b (см. рис. 31).

Взаимодействие двух атомов, имеющее вид

$$V = \frac{1}{R} - \frac{1}{r_{a2}} - \frac{1}{r_{b1}} + \frac{1}{r_{12}}$$

будем рассматривать как малое возмущение.

В первом приближении энергия взаимодействия двух атомов равна диагональному матричному элементу V, т. е.

$$\int \psi_0(r_{1a})\,\psi_0(r_{2b})\,V\dot{\zeta}_0(r_{1a})\,\psi_0(r_{2b})\,d\tau_1 d\tau_2,$$

где

$$\psi_0(r_{1a}) = 2e^{-r_{1a}}; \quad \psi_0(r_{2b}) = 2e^{-r_{2b}}.$$

В S-состоянии диагональные матричные элементы, т. е. среднее значение дипольного, квадрупольного и т. д. моментов, равны нулю, поэтому для вычисления энергии взаимодействия необходимо перейти ко второму приближению теории возмущений.

В операторе возмущения (1) ограничимся диполь - дипольным взаимодействием, как наиболее медленно убывающим с расстоянием. ДЛя получения оператора диполь - дипольного взаимодействия разложим потенциал V по убывающим степеням R. Разложение по шаровым функциям дает

$$\frac{1}{r_{l1}} = \frac{1}{|Rp - r_{1a}|} = \sum_{\lambda=0} \frac{r_{a1}^{\lambda}}{R^{\lambda+1}} P_{\lambda}(\cos\theta) =$$

$$= \frac{1}{R} + \frac{\boldsymbol{r}_{a1^p}}{R^2} + \frac{3\,(r_{a1p})^2 - \boldsymbol{r}_{a1}^2}{2R^3} + \cdots$$

$$\frac{1}{r_{12}} = \frac{1}{|Rp + r_{b2} - r_{a1}|} =$$

$$= \frac{1}{R} + \frac{(r_{a1} - r_{b2}, p)}{R^2} + \frac{3\,(r_{a1} - r_{b2}, \rho)^2 - (r_{a1} - r_{b2})^2}{2R^3} + \ldots$$

$$\frac{1}{r_{a2}} = \frac{1}{R} + \frac{(r_{b2}p)}{R^2} + \frac{3\,(r_{b2^p})^2 - r_{b2}^2}{2R^3} + \cdots$$

Подставляя полученные разложения в V, находим выражение для диполь - дипольного взаимодействия

$$V = -\frac{2z_1z_2 - x_1x_2 - y_1y_2}{R^3},$$

причем ось z направлена вдоль линии, соединяющей ядра. Как было уже сказано, среднее значение (2) по невозмущенной собственной функции $\psi = \psi_0(r_{a1})\,\psi_0(r_{b2})$ равно нулю. Недиагональные элементы (2), соответствующие переходам из основного состояния в возбужденные состояния, можно представить в виде

$$V_{00}^{mn} = -\frac{2z_{0m}z_{0n} - x_{0m}x_{0n} - y_{0m}y_{0n}}{R^3}.$$

На основании правила отбора матричные элементы z_{0n}, x_{0n}, y_{0n} отличны от нуля только для переходов из основного состояния в состояния

$$\psi_n(r)\cos\theta, \quad \psi_n(r)\sin\theta\cos\varphi,$$

причем все эти три матричные элемента равны друг другу. Энергия взаимодействия во втором приближении равна

$$E^{(2)} = \sum_{mn} \frac{\left(V_{00}^{mn}\right)^2}{2E_0 - E_m - E_n} = \frac{1}{R^6} \sum_{mn} \frac{4z_{0m}^2 z_{0n}^2 + x_{0m}^2 x_{0n}^2 + y_{0m}^2 y_{0n}^2}{2E_0 - E_m - E_n}$$

И.ПИ

$$E^{(2)} = \frac{6}{R^6} \sum_{mn} \frac{z_{0m}^2 z_{0n}^2}{2E_0 - E_m - E_n}.$$

Так как $E_0 < E_m$ и $E_0 < E_n$, то $E^{(2)}$ отрицательно и, следовательно, два атома в невозбужденном состоянии, находящиеся на большом расстоянии лруг от друга, притягиваются с силой, обратно пропорциональной седьмой степени расстояния. Для приближенного расчета суммы в (3) заметим, что разность энергий между различными верхними уровнями мала по сравнению с разностями энергий между верхними уровнями и основным. Поэтому приближенно (3) можно представить в виде

$$E^{(2)} = \frac{3}{R^6} \sum_m z_{0m}^2 \sum_n \frac{z_{0n}^2}{E_0 - E_n}.$$

Из теории квадратичного эффекта Штарка следует, что $\sum \frac{z_{0n}^2}{E_0 - E_n} = -\frac{1}{2}\alpha$, где α - поляризуемость атома. Для основного состояния атома водорода $x = 4,5$ ат. ед. При вычислении суммы $\sum\limits_{m\pm 0} z_{0m}^2$ воспользуемся правилом умножения матриц
(?)

$$(AB)_{nk} = \sum_m A_{nm} B_{mk}$$

$$\int \psi_n^* (AB)\psi_k d\tau = \sum_m \left\{ \int \psi_n^* A \psi_m^* d\tau \cdot \int \psi_m^* B \psi_k d\tau \right\}.$$

Положив в последнем соотношении $A = B = z, n = k = 0$, получим:

$$\left(z^2\right)_{00} = \sum_m z_{0m} z_{m0} = \sum z_{0nn}^2$$

И. ИИ

$$\sum_{m\neq 0} z_{0m}^2 = \sum_m z_{0m}^2 - z_{00}^2 = \left(z^2\right)_{00} - z_{00}^2.$$

Так как в S-состоянии в силу симметрии $z_{00} = 0$, а $\left(z^2\right)_{00} = \frac{1}{3}\left(r^2\right)_{00}$, то сумма

$$\sum_{m\neq 0} z_{0m}^2 = \frac{1}{3}\left(r^2\right)_{00} = 1$$

Таким образом, для $V(r)$ получаем окончательно выражение

$$V(R) = -\frac{6,75}{R^6}.$$

Для того чтобы уяснить, как могут возникнуть силы взаимодействия между двумя нейтральными сферически-симметричными атомами водорода, рассмотрим волновую функцию системы. Для волновой функции системы в первом приближении получаем выражение

$$\psi = \psi_0(r_{a1})\,\psi_0(r_{b2}) \left[1 + \frac{1}{2E_0 R^8}\left(x_1 x_2 + y_1 y_2 - 2z_1 z_2\right)\right].$$

Плотность вероятности $w(1,2)$, если пренебречь членами, содержащими $\frac{1}{R^6}$ в качестве множителя, имеет вид $w(r_{a1}, r_{b2}) = w_0(r_{a1})\,w_0(r_{b2}) \left[1 + \frac{1}{E_0 R^3}\left(x_1 x_2 + y_1 y_2 - 2z_1 z_2\right)\right]$ Если нет взаимодействия между атомами, плотность вероятности равна просто произведению $w(1)$ на $w(2)$, т. е. меж, положениями электронов в этом случае нет никакой корреляции. В случае же взаимодействия положение первого электрона не независимо от положения второго. Электроны занимают статистически чаще те положения, в которых их взаимная потенциальная энергия имеет по возможности меньшее значение.

Таким образом, силы взаимодействия в первом приближении можно объяснить не деформацией электронных оболочек, а корреляцией между положением электронов.

1+34

Докажем аддитивность для системы, состоящей из трех атомов. Из расчета будет видно, что его можно применить к любому числу атомов. Энергию взаимодействия запишем в следующей форме:

$$V = V(1,2) + V(2,3) + V(3,1),$$

где через $1, 2, 3$ обозначены совокупности координат первого, второго и третьего атомов. Мы рассматриваем взаимо- действие атомов, находящихся на большом расстоянии друг от друга; в этом случае обменные силы не играют никакой роли. Волновую функцию трех атомов при игнорировании обмена в нулевом приближении зададим в форме

$$\because = \bigcup_{ai}(1) \bigcup_{bk}(2) \uplus_{icl} (3),$$

где i, k, l - указывают квантовые состояния атомов a, b, c. Функции а (1), принадлежащие различным значениям i, ортогональны. То же самое можно сказать и про функции $\psi_{bk}(2), \psi_{cl}(3)$.

Энергия возмущения во втором приближении имеет вид

$$\varepsilon = V_{000}^{000} + \sum{}' \frac{|V_{ikl}^{000}|^2}{E_{a0} + E_{b0} + E_{c0} - E_{ai} - E_{bl} - E_{cl}}$$

Штрих у знака суммы означает, что i, k, l не должны одновременно равняться нулю. Первый член представляет классическое взаимодействие мультиполей. В нашем случае он равен нулю. В выражении (1) все члены, у которых одновременно $i \neq 0, k \neq 0, l \neq 0$, исчезают вследствие ортогональности функций.

Т ри частные суммы с $i = k = 0, l \neq 0; i = l = 0, k \neq 0$: $k = l = 0, i \neq 0$ означают поляризационные взаимодействия соответственно l-го, k-го и i-го атомов в результирующем поле двух огтальных атомов. В случае, когда распределение зарядов в атомах обладает шаровой симметрией, эти суммы также исчезают. Необходимо заметить, что эти суммы не могут быть получены путем аддитивного учета энергии взаимодействия каждой пары атомов. Нам остается рассмотреть те члены, в которых два индекса отличны от нуля. Итак, при сделанных предположениях относительно распределения заряда в атомах энергия взаимодействия может быть разложена на три частных суммы:

$$\varepsilon = \sum_{i\neq 0}{}' \frac{|V_{ik0}^{000}|^2}{E_{a0}+E_{b0}-E_{ai}-E_{bk}} + \underbrace{}_{b0}{}^{+E_{c0}-E_{bi}-E_{cl}} \sum_{k\neq 0 l\neq 0} + \sum_{i\neq 0 l\neq 0} \frac{|V_{0kl}^{000}|^2}{E_{a0}+E_{c0}-E_{ai}-E_{cl}}.$$

Вследствие ортогональности и нормированности собственных Функций атома матричный элемент

$$\begin{aligned} V_{ik0}^{000} &= \int \psi_{a0}^*(1)\psi_{b0}^*(2)\psi_{c0}^*(3) \cdot \{V(1,2)+ \\ &+ V(2,3) + V(3,1)\}\psi_{ai}^*(1)\psi_{bk}(2)\psi_{c0}(3)d\tau_1 d\tau_2 = \\ &= \int \psi_{a0}^*(1)\psi_{b0}^*(2)V(1,2)\psi_{ai}(1)\psi_{bk}(2)d\tau_1 d\tau_2 = \{V(1,2)\}_{ik}^{00} \end{aligned}$$

Следовательно, выражение (2) состоит из трех слагаемых, каждое из которых прдставляет дисперсионное взаимодействие пар атомов. Легко видеть, что этот расчет может быть распространен на произвольное число атомов.

В том случае, когда расстояния между атомами невелики, надо принять во внимание переходы электронов от одного атома к другому, т. е. принять во внимание обменныe силы.

18.1.13 Extra Problems about scattering 1

ГК-9.1. Медленное рассеяние притягателем

Найти сечение рассеяния частицы потенциальной ямои при малых скоростях (длина волны де Бройля значительно больше размеров ямы).

Solution

Потенциальная энергия частицы

$$\begin{aligned} U(r) &= -U_0 \quad (r < a), \\ U(r) &= 0 \qquad (r > a). \end{aligned}$$

Необходимо найти фазы рассеяния, т. е. асимптотический вид радиальных функций, удовлетворяющих уравнениям при

$$r > a \quad \chi_l'' + \left[k^2 - \frac{l(l+1)}{r^2}\right]\chi_l = 0, \quad k^2 = \frac{2\mu E}{\hbar^2},$$

при

$$r < a \quad \chi_l'' + \left[k'^2 - \frac{l(l+1)}{r^2}\right]\chi_l = 0, \quad k'^2 = \frac{2\mu\,(E+U_0)}{\hbar^2}$$

с граничным условием $\chi_l(0) = 0$.

В случае, когда длина волны де Бройля значительно больше размеров ямы, основной вклад в рассеяние вносит S-волна. Решение χ_0, удовлетворяющее граничному условию, имеет вид

$$\varkappa_0 = A\sin k'r (r < a),$$
$$\varkappa_0 = \sin\left(kr + \hat{\delta}_0\right)(r > a).$$

Фаза δ_0, также как и коэффициент A, определяется из условия непрерывности волновой функции и ее производной при $r = a$. Эти условия дают:

$$\delta_0 = \operatorname{arctg}\left(\frac{k}{k'}\operatorname{tg} k'a\right) - ka.$$

Итак, парциальное сечение для $l = 0$

$$\sigma_0 = \frac{4\pi}{k^2}\sin^2\delta_0 = \frac{4\pi}{k^2}\sin^2\left[\operatorname{arctg}\left(\frac{k}{k'}\operatorname{tg} k'a\right) - ka\right].$$

При малых скоростях падающих частиц ($k \to 0$) фаза рассеяния δ_0 пропорциональна k:

$$\delta_0 \approx k\left(\frac{\operatorname{tg} k_0 a}{k_0 a} - 1\right), \quad k_0^2 = \frac{2\mu U_0}{\hbar^2},$$

но благодаря множителю $\frac{1}{k^2}$ сечение σ_0 оказывается конечным

$$\sigma \approx 4\pi a^2\left(\frac{\operatorname{tg} k_0 a}{k_0 a} - 1\right)^2$$

(малые k).

Рассмотрим сечение 5_0 как функцию глубины ямы, которая характеризуется k_0. Если яма неглубока ($k_0 a \ll 1$), то

$$\sigma_0 = 4\pi a^2\frac{k_0^4 a^4}{9} = \frac{16\pi}{9}\frac{a^6 U_0^2\mu^2}{\hbar^4}.$$

Отметим, что согласно теории возмущений

$$f(\text{th}) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int U(r)d\tau = \frac{2\mu}{\hbar^2}U_0\frac{a^3}{3}$$

и, следовательно,

$$\sigma = 4\pi|f(\vartheta)|^2 = \frac{16\pi}{9}\frac{a^6 U_0^2\mu^2}{\hbar^4}.$$

По мере возрастания U_0 сечение возрастает и при $k_0 a = \frac{\pi}{2}$ становится неограниченно большим. Условие $k_0 a = \frac{\pi}{2}$ совпадает с условием появления в яме первого уровня. По мере углубления ямы сечение затем начинает уменьшаться и обращается в нуль при $\operatorname{tg} k_0 a = k_0 a$. При дальнейшем увеличении U_0 сечение продолжает колебаться между 0 и ∞, причем обращение сечения в ∞ наступает при появлении нового уровня в яме. Резкие колебания сечения при рассеянии медленных частиц качественно объясняет тот факт, что при рассеянии медленных электронов атомом сечение может значительно отличаться от геометрического.

Отметим, что если значение $k_0 a$ близко к целому кратному $\frac{\pi}{2}$, то формулы (2) и (3) необходимо видоизменить. Действительно, в этом случае $\operatorname{tg} \boldsymbol{k}'a$ оказывается большим числом и в формуле (1) нельзя произвести разложения, приводящего к формуле (7). В этом случае по-прежнему однако можно пренебречь слагаемым $ka \ll 1$ в квадратных скобках формулы (1). Тогда

$$\delta_0 = \operatorname{arctg}\left[\frac{k}{k'}\operatorname{tg} k'a\right]$$

и отсюда для сечения σ_0 получаем:

$$\sigma_0 = \frac{4\pi(1+O(xa))}{x^2+k^2},$$

где по условию

$$x = \frac{k'}{\operatorname{tg} k'a} \ll \frac{1}{a}.$$

Эта формула для «резонансного» рассеяния дает зависимость сечения от $\boldsymbol{k}$ при малых k, если потенциальная яма такова, что малым изменением ее глубины (или размера) можнодобиться появления или исчезновения дискретного уровня.

ГК-9.2. Медленное рассеяние отталкивателем

Определить сечение рассеяния медленных частиц в поле отталкивания

$$\begin{array}{ll} U(r) = U_0 & (r < a), \\ U(r) = 0 & (r > a). \end{array}$$

Solution

(??? по идее аналогично тому, что выше, понимал бы я это только!)

1+1

$0 = 4\pi a^2 \left(\frac{\operatorname{th} xa}{xa} - 1\right)^2$, где $\quad x = \frac{\sqrt{2\mu U_0}}{\hbar}$.

При $U_0 \to \infty \sigma = 4\pi a^2$, т. е. в 4 раза больше, чем сечение упругого рассеяния на непроницаемой сфере в классической механике.

ГК-9.3.

Выразить через фазы рассеяния первые три коэффициента разложения сечения упругого рассеяния $\frac{d\sigma}{d\Omega}$ по полиномам Лежандра.

Solution

3.
$$\begin{aligned} \frac{ds}{dQ} &= \frac{1}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\partial_l + \\ &+ \frac{6\cos\theta}{k^2}\sum_{l=0}^{\infty}(l+1)\sin\delta_l\sin\delta_{l+1}\cos(\delta_{l+1}-\delta_l) + \\ &+ \frac{5}{k^2}\frac{3\cos^2\vartheta-1}{2}\sum_{l=0}^{\infty}\left\{\frac{l(l+1)(2l+1)}{(2l-1)(2l+3)}\sin^2\delta_l + \right. \\ &\left. + \frac{3(l+1)(l+2)}{2l+3}\sin\delta_l\sin\delta_{l+2}\cos(\delta_{l+2}-\delta_l)\right\} + \ldots \end{aligned}$$

или

$$\int_0^{\pi} ds = \frac{4\pi}{k^2}\sum_{i=0}^{\infty}(2l+1)\sin^2 0_i$$

$$\int_0^{\pi}\cos\hat{\theta}d\sigma = \frac{8\pi}{k^2}\sum_{l=0}^{\infty}(l+1)\sin\hat{c}_l\sin\delta_{l+1}\cos(\delta_{l+1}-\delta_l)$$

$$\int_0^{\pi}\frac{3\cos^2\theta-1}{2}d\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}\frac{l(l+1)(2l+l)}{(2l+1)(2l+3)}\sin^2\delta_l +$$

$$+ \frac{12\pi}{k^2}\sum_{l=0}^{\infty}\frac{(l+1)(l+2)}{2l+3}\sin\delta_l\sin\delta_{l+2}\cos(\delta_{l+2}-\delta_l)$$

ГК-9.4.

Найти фазы рассеяния в поле $U = \frac{A}{r^2}$. Определить сечение рассеяния на малые углы.

Solution

1+3

Радиальные функции подчиняются уравнению

$$\chi_l'' + \left[k^2 - \frac{l(l+1)}{r^2} - \frac{2\mu A}{\hbar^2 r^2}\right]\chi = 0$$

и должны удовлетворять условиям $\chi_l(0) = 0$ и конечности при $r \to \infty$. Удовлетворяющее этим условиям решение имеет следующий вид:

$$\chi_{-l} = \sqrt{r} J_\lambda(kr),$$

где

$$\lambda = \sqrt{\left(l + \frac{1}{2}\right)^2 + \frac{2\mu \cdot A}{\hbar^2}}.$$

Из формул для асимптотического поведения $J_\lambda(kr)$ находим фазы:
$\delta_t = -\frac{\pi}{2}\left(\lambda - l - \frac{1}{2}\right) = -\frac{\pi}{2}\left\{\sqrt{\left(l+\frac{1}{2}\right)^2 + \frac{2\mu A}{\hbar^2}} - \left(l + \frac{1}{2}\right)\right\}$.
Независимость $\delta_{\mathrm{I}math}$ от k означает, что амплитуда рассеяния

$$f(\vartheta, k) = \frac{1}{k} f_0(\theta),$$

где $f_0(\vartheta)$ не зависит от энергии рассеиваемых частиц. Сечение рассеяния

$$d\tau = \frac{1}{k^2}|f_0(\ (?)\ |^2 dQ$$

обратно пропорционально энергии и характеризуется универсальным угловым распределением. Поскольку при $\to 0$ сумма, определяющая амплитуду рассеяния

$$f(i) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)\left[e^{2i}l - 1\right],$$

расходится, ясно, что для вычисления $f(\vartheta)$ при малых \$ существенны большие l. Для больших l имеем:

$$-\delta_l \approx -\frac{\pi\mu A}{(2l+1)\hbar^2} \ll 1,$$

юткуда

$$f(i) \approx \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)c_l \approx$$

$$\approx -\frac{\pi u \cdot A}{\hbar^2 k}\sum_{l=0}^{\infty}P_l(\cos i) = -\frac{\pi i \cdot A}{k\hbar^2}\frac{1}{2\sin\frac{\theta}{2}}.$$

В том случае, когда

$$\frac{8\mu A}{\hbar^2} \ll 1$$

выражение (1) для δ_l справедливо при любых l и таким образом для всех

$$f(\ \mathrm{ii}\ ) \approx -\frac{\pi\mu A}{k\hbar^2}\frac{1}{2\sin\frac{\vartheta}{2}},$$

$$ds = \frac{\pi^3 A^2}{2h^2 E}\operatorname{ctg}\frac{\vartheta}{2}d!$$

ГК-9.5.

Рассчитать дифференциальное сечение рассеяния в поле отталкивания $U = \frac{A}{r^2}$ в борновском приближении и согласно классической механике. Определить пределы применимости полученных формул.

Solution

Амплитуда рассеяния в борновском приближении имеет вид

$$f_{60_{\text{iA}}}(\hat{i}) = -\frac{\mu}{2\pi\hbar^2}\int e^{iqr}U(r)d\tau = -\frac{\pi_i A}{h^2 q},$$

где

$$\boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{k}, \quad q = 2\boldsymbol{k}\sin\frac{\vartheta}{2}.$$

Отсюда

$$d\sigma_{\text{born}} = |f(\text{th})^2|d\Omega = \frac{\pi^3\mu A^3}{2\hbar^2 E}\operatorname{ctg}\frac{\text{th}}{2}d\,\text{th}$$

В классической механике связь между углом рассеяния и прицельным параметром имеет вид

$$\int\limits_{i_0}^{\infty}\frac{\mu\nu p dr}{r^2\sqrt{2\mu(E-U)-\left(\frac{\mu\nu p}{r}\right)^2}} = \frac{\pi-\vartheta}{2},$$

где r_0 - корень подкоренного выражения. Производя интегрирование, находим:

$$p^2 = \frac{A}{E}\frac{1}{v}\frac{(\pi-\vartheta)^2}{2\pi-\vartheta},$$

откуда

$$d\tau = -2\pi\rho\frac{d\rho}{d\vartheta}d\theta = \frac{2\pi^3 A}{E}\frac{\pi-\vartheta}{\vartheta^2(2\pi-\vartheta)^2}d\theta.$$

При выполнении условия

$$\frac{8\mu A}{h^2} \ll 1$$

борновское приближение применимо для всех углов (ср. с предыдущей задачей).

В обратном предельном случае, если $\frac{8\mu A}{\hbar^2} \gg 1$ классическое выражение применимо для не слишком малых углов

$$0 \geqslant \frac{h^2}{8\mu A},$$

а для меньших углов

$$0 \leqslant \frac{\hbar^2}{8\mu A},$$

справедливы результаты расчета в борновском приближении.

ГК-9.6.

Найти дискретные уровни для частицы в поле притяжения $U(r) = -U_0 e^{-\frac{r}{a}}$ при $l = 0$. Определить фазу рассеяния δ_0 для этого потенциала и проанализировать связь между δ_0 и дискретным спектром.

Solution

1+5

Для радиальной функции имеем уравнение

$$\chi'' + \frac{2\mu}{\hbar^2}\left(E + U_0 e^{-\frac{r}{a}}\right)\chi = 0$$

Введем обозначения $k^2 = \frac{2\mu E}{\hbar^2}, x^2 = \frac{2\mu U_0}{\hbar^2}$ и в качестве независимой переменной выберем $\xi = e^{-\frac{r}{2a}}$. Решениями получающегося при этом уравнения

$$\chi'' + \frac{1}{\xi}\chi' + 4a^2\left(\frac{k^2}{\xi^2} + x^2\right)\chi = 0$$

являются бесселевы функции мнимого порядка $\chi = J_{\pm 2aki}(2a\chi\xi)$. Условие обращения χ в нуль при $r = 0$, т. е. при $\xi = 1$, приводит с точностью до нормировочной постоянной К выражению

$$\chi = J_{-2aki}(2ax)J_{2aki}\left(2ax^{\xi}\right) - J_{2aki}(2ax)J_{-2aki}\left(2ax^{\xi}\right).$$

Асимптотический вид Функции χ при $r \to \infty(\xi \to 0)$
$\chi = J_{-2aki}(2ax)\frac{e^{2aki\ln ax}}{\Gamma(2aki+1)}e^{-ikr} - J_{2aki}(2ax)\frac{e^{-2aki\ln ax}}{\Gamma(-2aki+1)}e^{ikr}$.

Коэффициенты при e^{-ikr} и e^{ikr} можно рассматривать как функции комплексного k. Если их обозначить через $a(k)$ и $b(k)$, то, как нетрудно убедиться, выполняются соотношения

$$a(-k) = -b(k),$$
$$a^*(k) = -b(k)$$

(при взятии комплексно-сопряженной величины k не заменяется на k^*).
Запишем асимптотическое выражение γ в виде

$$\chi = A\left(e^{-ikr - i\delta_0} - e^{ikr + i\delta_0}\right) = -2iA\sin(kr + \delta_0).$$

Фаза рассеяния δ_0 определяется из соотношения

$$e^{2i\delta_0} = \frac{J_{2aki}(2ax)}{J_{-2aki}(2ax)}\frac{\Gamma(2aki+1)}{\Gamma(-2aki+1)}e^{-4aki\ln ax}.$$

Связанному состоянию соответствует чисто мнимое значение $k = ik_n$ (в этом случае энергия отрицательна).

Для $k_n > 0$ коэффициент при $e^{-ikr} = e^k n^r$ в первом слагаемом асимптотического выражения для % должен обращаться в нуль. Таким образом, либо $J_{2ak_n}(2ax) = 0$, либо $\frac{1}{1(2ak_n+1)} = 0$. 11з второго условия следует:

$$2ak_n + 1 = -n \quad (n = 0, 1, 2, ...),$$

Т. е.

$$E = -\frac{\hbar^2 k_n^2}{2\mu} = -\frac{\hbar^2(n+1)^2}{8\mu a^2},$$

однако при этом индексы бесселевых функций становятся цельми чисіами и, так как $J_n(x) = (-1)^n J_{-n}(x)$, два реше- ния оказываются линейно зависимыми и волновая функция (1) обращается тождественно в нуль. Поэтому полученные уровни энергии являются фиктивными. Первое условие дает истинный дискретный спектр задачи:

$$J_{2ak}(2ax) = 0, \quad E_n = -\frac{\hbar^2 k_n^2}{2\mu}$$

Таким образом, нули выражения $e^{2i\delta_0(k)}$ лежат на мнимой оси и, помимо значений ik_n, соответствующих дискретным уровням (2), содержат лишние нули.

1+7

а) $d\sigma = \left(\frac{g^2}{2E}\right)^2 \frac{dQ}{\left(\sin^2\frac{\vartheta}{2} + \frac{\hbar^2\alpha^2}{2\mu E}\right)^2}$; $\quad \sigma = \frac{\pi\mu^2 g^4}{\hbar^2 a^2(2\mu E + \hbar^2 a^2)}$;
б) $d\sigma = \frac{\pi\mu^2 U_0}{4\hbar^4\alpha^6}e^{-\frac{4\mu\cdot E}{\hbar^2\alpha^2}\sin^2\frac{\theta}{2}}d\Omega$
$J = \frac{\pi^2 U_0^2\mu}{4\hbar^2\alpha^4 E}\left(1 - e^{-\frac{4\mu\cdot E}{\hbar^2\alpha^2}}\right)$
В) $ds = \frac{16\mu^2 U_0^2}{h^4}\frac{a^2}{(\alpha^2+q^3)^4}dQ$ $\sigma = \frac{64\pi}{3}\frac{\mu^2 U_0}{\hbar^4}\frac{16k^4+12k^2\alpha^2+3\alpha^4}{\alpha^4(\alpha^4+4k^2)^3}$

ГК-9.7.

Показать, что для кулоновского поля имеется однозначное соответствие между полюсами амплитуды рассеяния и уровнями дискретного спектра.

Указание. Воспользоваться формулой

$$e^{2i\grave{\partial}}l = \frac{\Gamma\left(l+1+\frac{l}{k}\right)}{\Gamma\left(l+1-\frac{i}{k}\right)}.$$

Solution

(решений нет, думай сам, или тупой.)

ГК-9.8.

Определить в борновском приближении дифференциальное и полное сечение рассеяния в поле а) $U(r) = g^2\frac{e^{-\alpha r}}{r}$, б) $U(r) = U_0 e^{-a^2 r^2}$, В) $U(r) = U_0 e^{-\alpha r}$.

Solution

ГК-9.9. Сечения на водороде и на гелии

Используя борновское приближение, найти дифференциальное и полное сечение упругого рассеяния быстрых электронов а) атомом водорода; б) атомом гелия.

9а)

(???? хорошая задача, подумаю потом!!)

Вычисляем атомный формфактор для водорода $F(q) = \int e^{iqv} n(r) d\tau = \frac{1}{\pi a^3}\int e^{iqr-\frac{2r}{a}} d\tau = \frac{1}{\left(1+\frac{q^2 a^i}{4}\right)^2}$ $\left(a = \frac{\hbar^2}{\mu e^2} -\right.$ боровский радиус).

Отсюда находим дифференциальное сечение

$$d\sigma = \frac{4a^2\left(8+q^2a^2\right)^2}{\left(4+q^2a^2\right)^4} d\Theta \quad \left(q = 2k\sin\frac{\theta}{2}\right)$$

и полное сечение

$$s = \frac{\pi a^2}{3}\frac{7k^4a^4+18k^2a^2+12}{\left(k^2a^2+1\right)^3}.$$

Условие применимости борновского приближения принимает в данном случае вид

$$ka \gg 1,$$

поэтому последняя формула упрощается

$$\sigma = \frac{7\pi}{3k^2}.$$

9 б)

Для атома гелия распределение плотности электронов, найденное с помощью вариационного расчета, имеет следующий вид:

$$n(r) = \frac{2}{\pi b^3} e^{-\frac{2r}{b}}, \quad b = \frac{16}{27}a.$$

Дифференциальное и полное сечение упругого рассеяния на атоме гелия в этом приближении имеет тот же вид, что и для рассеяния на атоме водорода. Нужно лишь в формулах (1) и (2) заменить a на b и ввести общий множитель $Z^2 = 4$. В частности,

$$\sigma = \frac{28\pi}{3k^3}.$$

ГК-9.10.

Рассмотреть столкновения одинаковых частиц с энергией взаимодействия $U(r)$. Найти эффективное сечение рассеяния медленных одинаковых частиц в случае короткодействующих сил.

Solution

ГК-9.11.

Рассчитать сечение упругого рассеяния электрона на электроне и α-частицы на α-частице.

Solution

ГК-9.12. Рассеяние нейтронов

Рассеяние нейтронов на протонах зависит от суммарного спина нейтрона и протона. При малых энергиях сечение в случае триплетного соотношения ($S = 1$) равно $\sigma^{\tau\ \text{трпл}} = 4\pi|f_3|^2 \approx 2 \cdot 10^{-24} c^2$, а в случае синглетного ($S = 0$)$\sigma^{\text{curl}} = 4\pi|f_1|^2 \approx 78 \cdot 10^{-24} cM^2$. Введем оператор

$$\hat{f} = \frac{f_1 + 3f_3}{4} + \frac{f_8 - f_1}{4} \left(\hat{\sigma}_n \hat{\sigma}_p\right).$$

Как легко видеть, в случаях триплетного и синглетного состояний его собственные значения равны f_3 и f_1 соответственно. Для того чтобы определить сечение рассеяния при произвольной поляризации нейтронов, необходимо усреднить оператор $\hat{f}^2$:

$$\sigma = 4\pi\overline{\hat{f}^2}.$$

Пусть спиновое состояние падающих нейтронов описывается функцией $\begin{pmatrix} e^{-ia}\cos\beta \\ e^{i\alpha}\sin\beta \end{pmatrix}$ (направление спина нейтрона задается полярными углами $A = 2\beta, \Phi = 2\alpha + \frac{\pi}{2}$; см. задачу 11§4), а спиновое состояние протонов функцией $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ (спины протонов направлены по оси z). Определить для этого случая сечение рассеяния нейтронов на протонах.

Solution

ГК-9.13.

Найти вероятность того, что рассеянный на протоне медленный нейтрон изменит ориентацию своего спина, если до столкновения спины нейтронов были направлены по оси z, а спины протонов - в противоположном направлении.

Solution

ГК-9.14.

Амплитуда рассеяния медленных нейтронов с энергиями заметно меньше тепловых $\left(\lambda > 10^{-8} c\mu\right.$, т. е. длина волны падающих нейтронов велика по сравнениго с взаимными расстояниями протонов в молекуле) на молекуле водорода равна сумме амплитуд для обоих протонов. Таким образом,

$$\hat{f} = \frac{f_1 + 3f_3}{2} + \frac{f_3 + f_1}{4} \left\{\hat{\sigma}_n \left(\hat{\sigma}_{p_1} + \hat{\sigma}_{p_v}\right)\right\}.$$

Протоны в молекуле водорода могут находиться как в состоянии с параллельными спинами (ортоводород), так и в состоянии с антипараллельными спинами (пароводород). Определить сечение рассеяния нейтронов на пароводороде и ортоводороде. 15. Определить полное сечение упругого рассеяния непроницаемоИ сферой радиуса a для быстрых частиц (длина волны де Бронля $\ll a$).

Solution

ГК-9.16.

Доказать следующие свойства амплитуды рассеяния при энергии $E \to 0$ (длины рассеяния): а) в поле отталкивания длина рассеяния отрицательна; б) в поле притяжения, если нет дискретных уровней, длина рассеяния положительна; в) длина рассеяния обращается в ∞, если при углублении потенциальной ямы появляется новый уровень. к эквивалентному интегральному уравнению ($E = 0$) то для асимптотического вида ψ получаем

$$\psi = 1 + \frac{a}{r},$$

где длина рассеяния

$$a = -\frac{\mu}{2\pi\hbar^2}\int \psi U d\tau$$

выражена через потенциальную энергию и $\psi_{E=0}$.

Solution

ГК-9.17.

Рассмотреть упругое рассеяние частиц со спином 1/2 на скалярной (спин равен нулю) частице. Найти дифференциальное сечение рассеяния с переориентацией спина. Рассмотреть рассеяние S и P волн.

18.1.14 Extra Problems about scattering 2

ГК-9.18. Известное разложение сечения в сумму двух (?????)

Доказать, что в общем случае неупругого рассеяния имеет место следующая формула, связывающая величину полсеяния при $0 = 0$

$$\sigma = \frac{4\pi}{k}\operatorname{Im} f(0).$$

Указание. Воспользоваться разложениями этих величин в ряды по орбитальному моменту:

$$f(i) = \frac{1}{2lk}\sum_{l=0}^{\infty}(2l+1)\left(\eta_l - 1\right)P_l(\cos i),$$

$$\sigma_{\text{ym}_\text{F}} = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)|1-\eta_l|^2,$$

$$\sigma_{\text{неупр}} = \frac{\pi}{k^2}\sum_{l=1}^{\infty}(2l+1)\left(1-|\Upsilon_l|^2\right).$$

Solution

ГК-9.19.

Рассмотрим предельный случай так называемого «черного» ядра. Радиус ядра R пусть будет велик в сравнении с де-бройлевской длиной волны нейтронов. Будем считать, что все нейтроны, попадающие в ядро, поглощаются. Определить полные сечения рассеяния и поглощения.

Solution

ГК-9.20.

Рассмотрим ядерную реакцию

$$A + a \to C \to B + b.$$

Как будет выглядеть угловое распределение продуктов ядерной реакции в системе центра инерции или, что то же саиое, в системе промежуточного ядра C в нижеперечисленшых случаях. Если равен нулю: а) спин промежуточного ядра; б) орбитальный момент относительного движения процуктов реакции; в) орбитальный момент относительного движения сталкивающихся тастиц (спин промежуточного ядра не равен чулю).

Solution

ГК-9.21.

Найти собственные функции операторэв квадрата и проекции полного изотопического спина I^2 и I_z системы нуклон—мезон *).

Solution

ГК-9.22.

В системе центра инерции рассеяние мезонов на нуклонах сводится к рассеянию частиц на неподвижном рассеивающем центре. Тогда вдали от центра падающая волна с определенным значением проекции спина S_z и проекции 'изотопического спина τ_z запишется в виде

$$e^{ikz}\begin{pmatrix}1\\0\end{pmatrix}\text{ò}\ (\pi-\pi_i)\,\delta\,(n-\tau_z)\,.$$

Здесь π_i принимает значения:

$$\begin{array}{ll}\pi_i=1 \text{ для } \pi^+\text{-мезона}, & \delta(\pi-1)=\varphi_+,\\ \pi_i=0 \text{ для } \pi^0\text{-мезона}, & \delta(\pi)=\varphi_0,\\ \pi_i=-1 \text{ для } \pi^-\text{-мезона}, & \delta(\pi+1)=\varphi_-,\end{array}$$

τ_z принимает значения:

$$\tau_z=\frac{1}{2}\text{ для протона}, \qquad \delta\left(n-\frac{1}{2}\right)=\psi_p,$$

$$\tau_z=-\frac{1}{2}\text{ для нейтрона}, \qquad \delta\left(n+\frac{1}{2}\right)=\psi_n.$$

Разложить падающую волну по собственным функциям операторов J^2, J_z, I^2, I_z.

Указание. В системе мезон-нуклон интегралами движения являются четн зсть $(-1)^l$, полный момент J, изотопический спин I.

Так как полный спин в такой системе равен $\frac{1}{2}$, то сохраняется также и орбитальный момент l. ПJэтому при разложении палающей волны по собственным функциям операторов сохраняющихся величин можно вместо суммирования по J, I суммировать по l, I.

Solution

ГК-9.23. Сечения пи мезонов на протонах через фазы

Найти амплитуды рассеяния π-мезонов на нуклонах, выраженные через фазы, для следующих реакции:

$$\pi^+ + p \to \pi^+ + p,$$
$$\pi^- + p \to \pi^- + p,$$
$$\pi^- + p \to \pi^0 + n.$$

Solution

ГК-9.24. Амплитуды для разных реакций (??????)

Показать, что амплитуды рассеяния для всех возможных реакций мезона с нуклоном выражаются через написанные в задаче 23 в силу гипотезы об изотопической инвариантности.

Выразить их через амплитуды рассеяния для состояний с изотопическим спином 3/2 и 1/2.

Solution

ГК-9.25. Полные сечения пи мезонов на протонах через фазы

Выразить через фазы полные сечения реакций:

$$\pi^+ + p \to \pi^+ + p,$$
$$\pi^- + p \to \pi^- + p,$$
$$\pi^- + p \to \pi^0 + n.$$

(???? в чем отличие от просто 9.23, не то же самое там???)

Solution

ГК-9.26.

В области малых энергий, когда длина волны мезона значительно больше радиуса сил взаимодействия между мезоном и нуклоном, основной вклад в рассеяние вносят лишь S и P-волны.

Найти дифференциальное сечение рассеяния, выраженное через фазы, для реакций:

$$\pi^+ + p \to \pi^+ + p,$$
$$\pi^- + p \to \pi^- + p,$$
$$\pi^- + p \to \pi^0 + n.$$

Solution

ГК-9.27. π-мезоны на поляризованных протонах

Пучок π-мезонов рассеивается на неполяризованной мишени из протонов, т. е. в мишени число протонов с $S_z = 1/2$ равно числу протонов с $S_z = -1/2$. Оказывается, что при рассеянии неполяризованные вначале протоны поляризуются. Определить величину поляризации протонов, учитывая только S - и P-волны.

Solution

10

1+9

Волновая функция системы из двух одинаковых частиц имеет вид произведения орбитальной и спиновой функций: Независимо от того, является ли спин частиц целым или полущелым, четному суммарному спину соответствует симметричная орбитальная волновая функция, а нечетному-антисимметричная.

После перехода к системе центра инерции и отделения переменной центра тяжести орбитальная волновая функция принимает вид.

$$\Psi\left(r_1, r_2\right) = \varphi(R)\psi(p),$$

где

$$R = \frac{\boldsymbol{r}_1 + \boldsymbol{r}_2}{2}, \quad p = \boldsymbol{r}_1 - \boldsymbol{r}_2.$$

При замене $\boldsymbol{r}_1$ на $\boldsymbol{r}_2$ функция $\varphi(R)$, опигывающая движение центра тяжести, очевидно, не меняется. Таким образом, волновая функция отногительного движения двух частиц должна быть четной

$$\psi(p) = \psi(-p)$$

в том случае, если суммарный спин S четен, и нечетной

$$\psi(p) = -\psi(-p),$$

если спин S нечетен.

Невозмущенную волновую функцию можно записать в виде

$$\psi(\rho) = e^{i\pi_{0p}} + e^{-ik_{op}p},$$

если S - четное, и

$$\psi(\rho) = e^{ik_0\rho} - e^{-ik_0\rho},$$

если S - нечетное. В результате взаимодействия частиц возникает рассеянная волна $\frac{F(\vartheta)}{\rho}e^{ikp}$, где ϑ-угол между $\boldsymbol{k}_0$ и направлением, в котором разлетаются частицы в системе центра инерции. Амплитуду рассеяния можно выразить через амплитуду рассеяния частицы с массой, равной приведенной массе обеих частиц в поле $U(r)$. Действительно, $\psi(\rho)$ удовлетворяет уравнению

$$\left\{-\frac{\hbar^2}{\mu}\left(\Delta_p + k^2\right) - U(p)\right\} \backsim (p) = 0.$$

Если падающей волне $e^{ik_p\rho}$ соответствует рассеянная $\frac{f(\vartheta)}{r}e^{ik\rho}$, то для падающей волны (1)

$$F_0(i) = f(i) + f(\pi -) \quad \text{(спин четен)},$$

а для (2)

$$F_1(\vartheta) = f(\vartheta) - f(\pi - \vartheta) \text{ (спин нечетен)}.$$

Вероятность рассеяния одной из частиц в телесном угле dQ (при этом другая частица движется в противоположном направлении), отнесенная к плотности падающего потока:

$$d\tau_0 = |f(9) + f(\pi - \vartheta)|^2,$$
$$d\sigma_1 = |f(\vartheta) - f(\pi - \vartheta)|^2.$$

Амплитуда $f(0)$ выражается через фазы рассеяния δ_l по формуле

$$f(\vartheta) = \frac{1}{2lk}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)\left[e^{2i\hbar}l - 1\right].$$

Принимая во внимание, что

$$P_l(\cos(\pi - \vartheta)) = P_l(-\cos\vartheta) = (-1)^l P_l(\cos\vartheta),$$

Находим:

$$F_0(i) = \frac{1}{lk}\sum_{\text{четные } l}(2l+1)P_{\text{Im}ath}(\cos i)\left[e^{2\dot{i}}l - 1\right],$$
$$F_1(i) = \frac{1}{ik}\sum_{\text{нечетные Im}ath}(2l+1)P_l(\cos i)\left[e^{2i\delta}l - 1\right].$$

Для медленных частиц наибольший вклад в рассеяние вносят малые l. В случае четного суммарного спина сечение (как и при рассеянии различных частиц) сферически симметрично и не обращается в нуль при $k \to 0$.

Если же суммарный спин нечетный, то сечение определяется членом с $l = 1$. Поскольку $\delta_l \sim k^{2l+1}$ для малых волновых чисел k, сечение обращается в нуль как E^2 (при $E \to 0$) и имеет угловую зависимость $\sim \cos^2\vartheta$.

11

В случае кулоновского поля амплитуда рассеяния

$$f(\vartheta) = -\frac{1}{2k^2\sin^2\frac{\vartheta}{2}}e^{-\frac{2i}{k}\ln\sin\frac{\theta}{2}\Gamma\left(1+\frac{l}{k}\right)}\frac{\Gamma\left(1+\frac{l}{k}\right)}{\Gamma\left(1-\frac{l}{k}\right)}.$$

Воспользовавшись результатом предыдущей задачи, находим дифференциальное сечение рассеяния в случае четного спина

$$d\sigma_0 = |f(n) + f(\pi - n)|^2 dQ = \frac{1}{4k^4}\left\{\frac{1}{\sin^4\frac{\theta}{2}} + \frac{1}{\cos^4\frac{\theta}{2}} + \frac{2\cos\left(\frac{2}{k}\ln\text{tg}\frac{\theta}{2}\right)}{\sin^2\frac{9}{2}\cos^2\frac{8}{2}}\right\}d\Omega.$$

Эта формула дает сечение рассеяния α-частиц, у которых спин равен нулю.

В случае двух электронов возможно состояние с суммарным спином 1. Тогда дифференциальное сечение

$$d\sigma_1 = |f(7) - f(\pi - \vartheta)|^2 = \frac{1}{4k^4}\left\{\frac{1}{\sin^4\frac{7}{2}} + \frac{1}{\cos^4\frac{\pi}{2}} - \frac{2\cos\left(\frac{2}{k}\ln\text{tg}\frac{\theta}{2}\right)}{\sin^2\frac{9}{2}\cos^2\frac{8}{2}}\right\}d\Omega.$$

Если рассеивающиеся электроны не поляризованы, то возможны три значения проекции суммарного спина вдоль некоторого направления $z : S_z = 0, S_z = 1, S_z = -1$ и два значения полного спина $S = 0$ и $S = 1$. Вероятность каждого из значений проекций $W_{-1} = \frac{1}{4}, W_0 = \frac{1}{2}, W_{+1} = \frac{1}{4}$. Значения $S_z = +1$ или $S_z = -1$ соответствуют непременно полному спину $S = 1$. Поскольку различные значения проекции для $S = 1$ равновероятны, то вероятность $S_z = 0$ при полном спине 1, так же как и для $S_z = \pm 1$, равна $\frac{1}{4}$. Таким образом, вероятность того, что полный спин $S = 0$, равна $w_0 - \frac{1}{4} = \frac{1}{4}$, а вероятность $S = 1$ равна $\frac{3}{4}$. Поэтому для неполяризованных пучков электронов

$$ds = \frac{1}{4}d\sigma_0 + \frac{3}{4}ds_1 = \\ = \frac{1}{4k^4}\left\{\frac{1}{\sin^4\frac{\theta}{2}} + \frac{1}{\cos^4\frac{\theta}{2}} - \frac{\cos\left(\frac{2}{k}\ln\mathrm{tg}\,\frac{\theta}{2}\right)}{\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2}}\right\}dQ.$$

Последний интерференционный член в фигурных скобках характерен для рассеяния тождественных частиц. При $\hbar \to 0$ формула для $d\sigma$ должна переходить в классическую формулу Резерфорда, которая для системы центра инерции имеет вид

$$ds = \frac{1}{4k^4}\left\{\frac{1}{\sin^4\frac{\%}{2}} + \frac{1}{\cos^4\frac{9}{2}}\right\}d\Omega.$$

Переход этой формуле происходит необычно. При выполнении условия $\frac{e^2}{\hbar v} \gg 1$, когда применимо классическое рассмотрение, интерференционный член, имеющий в обычных единицах вид

$$\frac{\cos\left(\frac{2e^2}{\hbar v}\ln\mathrm{tg}\,\frac{\vartheta}{2}\right)}{\sin^2\frac{\theta}{2}\cos^2\frac{\vartheta}{2}}$$

быстро осциллирует. Таким образом, квантовое дифференциальное сечение для строго фиксированного 7 существенно отличается от классического даже для больших значений $\frac{e^2}{\hbar\bar{v}}$. Однако при усреднении по небольшому интервалу углов $\Delta i \sim \frac{\hbar v}{e^2}$ интерференционный член обращается в нуль и квантовая формула переходит в классическую.

12.

$$\hat{f}^2 = \frac{3}{4}f_3^2 + \frac{1}{4}f_1^2 + \frac{1}{4}\left(f_3^2 - f_1^2\right)\left(\hat{\sigma}_n\hat{\sigma}_p\right).$$

Среднее значение оператора $(\hat{\sigma}_n\hat{\sigma}_p)$ в состоянии, характеризуемом спиновой Фуункцией равно

$$\begin{pmatrix} e^{-i\alpha}\cos\beta \\ e^{i\alpha}\sin\beta \end{pmatrix}_n \begin{pmatrix} 1 \\ 0 \end{pmatrix}_p,$$

$$\overline{\left(\hat{\sigma}_n\hat{\sigma}_p\right)} = \cos^2\beta - \sin^2\beta.$$

Таким образом, для сечения рассеяния находим выражение

$$\sigma = \pi\left\{3f_3^2 + f_1^2 - \left(f_3^2 - f_1^2\right)\cos 2\beta\right\}$$

HI

$$\sigma = \left\{\frac{3}{4}\sigma^{\text{трипл}} + \frac{1}{4}\sigma^{\text{сингл}} - \frac{\cos 2\beta}{4}\left(\sigma^{\text{Ti ипл}} - \sigma^{\text{сингл}}\right)\right\}.$$

В случае неполяризованного пучка нейтронов сечение равно

$$\sigma = \frac{3}{4}\sigma^{\text{ti ипл}} + \frac{1}{4}\sigma^{\text{сингл}},$$

поскольку $\overline{\cos 2\beta} = 0$.

13

Спиновое состояние нейтрона и протона до взаимодействия описывается Функцией

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}_n \begin{pmatrix} 0 \\ 1 \end{pmatrix}_p.$$

Эту функцию разложим по спиновым функциям синглетного и триплетного состояний

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}_n \begin{pmatrix} 0 \\ 1 \end{pmatrix}_p = \frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2}}\left\{\begin{pmatrix} 1 \\ 0 \end{pmatrix}_n \begin{pmatrix} 0 \\ 1 \end{pmatrix}_p + \begin{pmatrix} 0 \\ 1 \end{pmatrix}_n \begin{pmatrix} 1 \\ 0 \end{pmatrix}_p\right\} + \right.$$

$$\left. + \frac{1}{\sqrt{2}}\left\{\begin{pmatrix} 1 \\ 0 \end{pmatrix}_n \begin{pmatrix} 0 \\ 1 \end{pmatrix}_p - \begin{pmatrix} 0 \\ 1 \end{pmatrix}_n \begin{pmatrix} 1 \\ 0 \end{pmatrix}_p\right\}\right].$$

Рассеянная волна имеет вид
или

$$\frac{e^{ikr}}{r}\frac{1}{\sqrt{2}}\left[f_3\frac{1}{\sqrt{2}}\left\{\begin{pmatrix}1\\0\end{pmatrix}_n\begin{pmatrix}0\\1\end{pmatrix}_p+\begin{pmatrix}0\\1\end{pmatrix}_n\begin{pmatrix}1\\0\end{pmatrix}_p\right\}+\right.$$
$$\left.+f_1\frac{1}{\sqrt{2}}\left\{\begin{pmatrix}1\\0\end{pmatrix}_n\begin{pmatrix}0\\1\end{pmatrix}_p-\begin{pmatrix}0\\1\end{pmatrix}_n\begin{pmatrix}1\\0\end{pmatrix}_p\right\}\right]$$
$$\frac{e^{ikr}}{r}\left\{\frac{f_3+f_1}{2}\begin{pmatrix}1\\0\end{pmatrix}_n\begin{pmatrix}0\\1\end{pmatrix}_p+\frac{f_3-f_1}{2}\begin{pmatrix}0\\1\end{pmatrix}_n\begin{pmatrix}1\\0\end{pmatrix}_p\right\}$$

отсюда следует, что вероятность переориентации равна

$$\frac{1}{2}\frac{(f_3-f_1)^2}{f_3^2+f_1^2}.$$

14

Введем оператор суммарного спина двух протонов

$$\frac{1}{2}\left(\hat{\sigma}_{p_1}+\hat{\sigma}_{p_2}\right)=\hat{\boldsymbol{S}}.$$

Как пегко показать,

$$\left(\hat{\sigma}_n\hat{S}^2=\hat{S}^2-\left(\hat{\sigma}_n\hat{S}\right).\right.$$

С. учетом последнего соотношения выражение для $\hat{f}^2$ примет вид
$\hat{f}^2=\frac{1}{4}\left\{(f_1+3f_3)^2+\left(5f_3^2-2f_3f_1-3f_1^2\right)\left(\hat{\sigma}_n\hat{\boldsymbol{S}}\right)+(f_3-f_1)^2\hat{\boldsymbol{S}}^2\right\}$
В случае рассеяния на параводороде сечение равно

$$\sigma^{\text{papa}}=\pi\left(f_1+3f_3\right)^2.$$

Естественно, что это сечение не зависит от поляризации падающих нейтронов, поскольку нет физически выделенного направления в пространстве.
Сечение рассеяния на ортоводороде равно
$\sigma^{\text{or ro}}=\pi\left\{(f_1+3f_3)^2+\right.$

$$\left.+\left(5f_3^2-2f_3f_1-3f_1^2\right)\cos 2\beta+2\left(f_3-f_1\right)^2\right\}$$

где 2β - угол между направлениями суммарного спина двух протинов и спина нейтрона.
Если пучок нейтронов не поляризован, то среднее значение $\cos 2\beta$ по смешанному ансамблю равно нулю и σ° примет вид

$$\sigma^{\text{орто}}=\pi\left\{(f_1+3f_3)^2+2\left(f_3-f_1\right)^2\right\},$$

а отношение сечений будет равно

$$\frac{\sigma^{\text{орто}}}{\sigma^{\text{пог'}}}=1+2\left(\frac{f_3-f_1}{f_1+3f_3}\right)^2$$

15

1+14

Радиальные функции, удовлетворяющие граничному условию $\chi_l(a)=0$, выражаются следующим образом через бесселевы функции:

$$\chi_l=\sqrt{r}\left\{J_{-l-1/2}(ka)J_{l+1/2}(kr)-J_{l+1/2}(ka)J_{-l-1/2}(kr)\right\}$$

Из формул для асимптотического поведения бесселевых Функций находим фазы рассеяния

$$\operatorname{ctg}\delta_l=(-1)^{\mathrm{Im}ath+1}\frac{J_{-l-1/2}(ka)}{J_{l+1/2}(ka)}.$$

Отсюда полное сечение упругого рассеяния

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l-1)\frac{J^2_{l+l_{i,2}}(ka)}{J^2_{l+1,2}(ka)+J^2_{-l-1,2}(ka)} \approx 2\pi a^2.$$

17

1+16

На больших расстояниях от мишени (мишень состоит из скалярных частиц) волновая функция падающих частиц имеет вид

$$e^{ikz}\begin{pmatrix}1\\0\end{pmatrix} = \frac{1}{2kr}\sum_{l=0}^{\infty} i^{l+1}(2l+1)\begin{pmatrix}1\\0\end{pmatrix}P_l(\cos v)\times$$
$$\times\left\{e^{-i\left(kr-\frac{\pi l}{2}\right)} - e^{i\left(kr-\frac{\pi l}{2}\right)}\right\}.$$

Разложим функцию $\begin{pmatrix}1\\0\end{pmatrix}P_l(\cos\vartheta)$ по собственным функциям оператора $\hat{J}^2$. В результате разложения получим:

$$\begin{pmatrix}1\\0\end{pmatrix}P_l(\cos\theta) = \frac{2\sqrt{\pi}}{\sqrt{2l+1}}\begin{pmatrix}1\\0\end{pmatrix}Y_{l0}(\theta) =$$
$$= \frac{2\sqrt{\pi}}{2l+1}\left\{\sqrt{l+1}\Psi_l^+ + \sqrt{l}\Psi_l^-\right\}.$$

Здесь через Ψ_l^+и Ψ_l^-мы обозначили функции Паули

$$\Psi_l^+ = \frac{1}{\sqrt{2l+1}}\begin{pmatrix}\sqrt{l+1}Y_{l0}\\ \sqrt{l}Y_{l1}\end{pmatrix}\quad\left(j=l+\frac{1}{2},l,j_z=\frac{1}{2}\right),$$
$$\Psi_l^- = \frac{1}{\sqrt{2l+1}}\begin{pmatrix}\sqrt{lY_{l0}}\\ -\sqrt{l+1}Y_{21}\end{pmatrix}\quad\left(j=l-\frac{1}{2},l,j_z=\frac{1}{2}\right)$$

(см. задачу 20§4).
Подставляя (2) в (1), имеем:

$$e^{ikz}\begin{pmatrix}1\\0\end{pmatrix} \approx \frac{\sqrt{\pi}}{kr}\sum_{l=0}^{\infty} i^{l+1}\left\{\sqrt{l+1}\Psi_l^+ + \sqrt{l}\Psi_l^-\right\}\times$$
$$\times\left\{e^{-\left(kr-\frac{\pi l}{2}\right)} - e^{i\left(kr-\frac{\pi l}{2}\right)}\right\}.$$

В результате взаимодействия изменится только расходящаяся волна $\frac{e^{ikr}}{r}$.

Так как при любом законе взаимодействия этих частиц $\hat{j}^2, \hat{l}^2$ и $\hat{j}_z$ будут интегралами движения (см. задачу 39§4), то изменение в общем случае будет различно для состояний с различными квантовыми числами j, l. Для рассеянной волны получим выражение следующего вида:

$$\Psi_s \approx \frac{e^{ikr}}{r}\frac{\sqrt{\pi}}{ik}\sum_{l=0}^{\infty}\left\{\sqrt{l+1}\left(\eta_l^+ - 1\right)\Psi_l^+ + \sqrt{l}\left(\eta_l - -1\right)\Psi_l^-\right\},$$
$$\eta_l^+ = \eta\left(j=l+\frac{1}{2},l\right),$$
$$\eta_l^- = \eta\left(j=l-\frac{1}{2},l\right)$$

или $\Psi_8 \approx \frac{e^{ikr}}{r}\frac{\sqrt{\pi}}{ik}\sum\limits_{l=0}^{\infty}\frac{1}{\sqrt{2l+1}}\times$
$X\left\{\begin{pmatrix}1\\0\end{pmatrix}Y_{l0}\left[(l+1)\left(\eta_l^+-1\right)+l\left(\eta_i--1\right)\right]+\begin{pmatrix}0\\1\end{pmatrix}Y_{l1}\left(\eta_l+-\eta_l-\right)\right\}$

Отсюда видно, что переориентация спина частицы может произойти в том случае, когда $r_l^+ \neq \eta_i^-$. Выразим сечение рассеяния через η_i^+и η_i^-.

Дифференциальное сечение рассеяния с изменением поляризации $d\sigma_1$ равно

$$d\sigma_1 = \frac{\pi}{k^2}|\sum_{l=0}^{\infty}\sqrt{\frac{l(l+1)}{2l+1}}\left(\eta_l + ...\eta_l^-\right)Y_{l1}|^2 dQ,$$

а сечение $d\sigma_2$ без изменения поляризации равно $d\sigma_2 = \frac{\pi}{k^2}|\sum\limits_{l=0}^{\infty}\frac{1}{\sqrt{2l+1}}Y_{l0}\left\{(l+1)\left(\eta_l^+ - 1\right) + l\left(\eta_l^- - 1\right)\right\}|^2 dQ$.

Когда относительная скорость частиц не велика, нужно принимать во внимание рассеяния только S - и P-волн

$$\left(|\eta_l^+ - 1| \ll 1, \quad |\eta_l^- - 1| \ll 1, \quad \text{если} \quad l > 1\right).$$

В этом случае

$$d\sigma_1 \approx \frac{1}{4k^2}\left(\eta_1^+ - \eta_1\right)\sin^2\theta d\Omega,$$
$$d\sigma_2 \approx \frac{1}{4k^2}|\cos\vartheta\left(2\eta_1^+ + \eta_1^- - 1\right) + \eta_0^+ - 1|^2 d\Omega.$$

Из выражения для $d\sigma_1$ видно, что частицы, изменившие ориентацию спина, рассеиваются главным образом в направлении, перпендикулярном оси z.

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1+18

Поскольку $R \gg \lambda$, то можно применять квазиклассические соображения. В ядро попадают все частицы с $l \leqslant \frac{R}{\pi}$, следовательно,

$$\eta_l = 0 \text{ для} \quad l < \frac{R}{\lambda},$$
$$r_{il} = 1 \quad \text{для} \quad l > \frac{R}{\lambda}.$$

Подставляя значение η_l в выражение для полных сечений $\sigma_r = \pi\lambda^2\sum(2l+1)\left(1 - |\eta_l|^2\right)$, $\sigma_s = \pi\lambda^2\sum(2l+1)|1-\eta_{il}|^2$, имеем:

$$\sigma_r = \sigma_s = \pi\lambda\sum_{l=0}^{\frac{R}{\lambda}}(2l+1) \approx \pi R^2.$$

Таким образом, полное сечение $\sigma = \sigma_r + \sigma_s$ равно удвоенному геометрическому сечению ядра.

20

Во всех трех случаях распределение изотропно.

21

Собственные функции оператора I_z для системы мезон - нуклон записываются как всевозможные произведения функций φ и (???). При этом, φ относится различным зарядовым состояниям мезона $(\varphi_+, \varphi_0, \varphi_-)$, а у нуклона $\left(\bigsqcup_p, \iota_n\right)$. Всего таких фуикций будет шесть:

$(p^+) = \varphi_+\psi_p$ $I_z = \frac{3}{2}$	$(p^0) = \varphi_0\psi_p$ $I_z = \frac{1}{2}$	$(p^-) = \varphi_-\psi_p$ $I_z = -\frac{1}{2}$
$(n^+) = \varphi_+\psi_n$ $I_z = \frac{1}{2}$	$(n^0) = \varphi_0\psi_n$ $I_z = -\frac{1}{2}$	$(n^-) = \varphi_-\psi_n$ $I_z = -\frac{3}{2}$

Здесь (p^+)обозначает функцию системы, составленной из π^+-мезона и протона; (n^+)- функцию, составленную из π^+-мезона и нейтрона и т. д. Эти функции, вообще говоря, не являются собственными функциями оператора квадрата полного изотопического спина системы I^2.

Собственные функции I^2, одновременно принадлежащие заданному I_z, будут линейными комбинациями из вышенаписанных функций, взятых с коэффициентами Клебша - Жордана. Коэффициенты Клебша – Кордана для $m' = \pm 1/2$ имеют вид (см. задачу 20§4)

	$m'=\frac{1}{2}$	$m'=-\frac{1}{2}$
$I=j+\frac{1}{2}$	$\sqrt{\frac{j+M+\frac{1}{2}}{2j+1}}$	$\sqrt{\frac{j-M+\frac{1}{2}}{2j+1}}$
$I=j-\frac{1}{2}$	$-\sqrt{\frac{j-M+\frac{1}{2}}{2j+1}}$	$\sqrt{\frac{j+M+\frac{1}{2}}{2j+1}}$

В нашем случае $M=I_z, j=1, m'=\tau_z$.
Пользуясь этой таблицей, получаем собственные функции $\Phi^I_{I_z}$ операторов I^2 и I_z:

$$\Phi^{3/2}_{3/2}=\left(p^+\right),$$
$$\Phi^{3/2}_{1/2}=\sqrt{\frac{2}{3}}\left(p^0\right)+\sqrt{\frac{1}{3}}\left(n^+\right)$$
$$\Phi^{3/2}_{-1/2}=\sqrt{\frac{1}{3}}\left(p^-\right)+\sqrt{\frac{2}{3}}\left(n^0\right),$$
$$\Phi^{3/2}_{-3/2}=\left(n^-\right),$$
$$\Phi^{1/2}_{1/2}=-\sqrt{\frac{1}{3}}\left(p^0\right)+\sqrt{\frac{2}{3}}\left(n^{-1}\right),$$
$$\Phi^{1/2}_{-1/2}=-\sqrt{\frac{2}{3}}\left(p^-\right)+\sqrt{\frac{1}{3}}\left(n^0\right).$$

Отсюда легко выразить собственные функции системы мезон - нуклон через собственные функции I^2 и I_z. Они оказываются равными:
$(p^+)=\Phi^{3/2}_{2/2}, \quad (n^+)=\sqrt{\frac{1}{3}}\Phi^{3/3}_{1/2}+\sqrt{\frac{2}{3}}\Phi^{1/2}_{1,2},$
$\left(p^0\right)=\sqrt{\frac{2}{3}}\Phi^{3/2}_{1/2}-\sqrt{\frac{1}{3}}\Phi^{1/2}_{1/2}, \left(n^0\right)=\sqrt{\frac{2}{3}}\Phi^{3/2}_{-1/2}+\sqrt{\frac{1}{3}}\Phi^{1/2}_{-1/2},$
$(p^-)=\sqrt{\frac{1}{3}}\Phi^{3/2}_{-1/2}\cdots\sqrt{\frac{2}{3}}\Phi^{1/2}_{-1/2}, \quad (n^-)=\Phi^{3/2}_{-3/,\cdot}$

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Разложение падающей волны имеет вид

$$\psi=e^{ikz}\begin{pmatrix}1\\0\end{pmatrix}\delta\left(\pi-\pi_i\right)\delta\left(n-\tau_z\right)=$$
$$=\sum_{l=0}^{\infty}il(2l+1)P_l(\cos\theta)\begin{pmatrix}1\\0\end{pmatrix}\delta\left(\pi-\pi_i\right)\delta\left(n-\tau_z\right)\frac{\sin\left(kr-\frac{\pi l}{2}\right)}{kr}=$$
$$=2\sqrt{\pi}\sum_{l=0}^{\infty}\sum_{I}^{\infty}C^{I\tau}_{I}\Phi^I_z I_z i^l\sqrt{2l+1}Y_{l0}\begin{pmatrix}1\\0\end{pmatrix}\frac{\sin\left(kr-\frac{\pi l}{2}\right)}{kr}$$

где $C^{I\tau}_{I^I_z}$ - коэффициенты Клебша - Жордана, определяемые из таблицы

	$\tau_z=\frac{1}{2}$	$\tau_z=-\frac{1}{2}$
$C^{3/2}_{I^3_z}$	$\sqrt{\frac{1}{2}+\frac{I_z}{3}}$	$\sqrt{\frac{1}{2}-\frac{I_z}{3}}$
$C^{1/2}_{\frac{1}{z}}$	$-\sqrt{\frac{1}{2}-\frac{I_z}{3}}$	$\sqrt{\frac{1}{2}+\frac{I_z}{3}}$

Здесь мы учли, чго (см. задачу 21)

$$\delta\left(\pi-\pi_i\right)\delta\left(n-\tau_z\right)=\sum_I C^{I\tau_z}_I\Phi^I_{I_z}$$

Введем функции Паули для $m_j=1/2$ (см. задачу 17 §9):

$$Y^+_l=\begin{pmatrix}\sqrt{\frac{l+1}{2l+1}}Y_{l0}\\ \sqrt{\frac{l}{2l+1}}Y_{l1}\end{pmatrix}; \quad Y^-_l=\begin{pmatrix}\sqrt{\frac{l}{2l+1}}Y_{l0}\\ \sqrt{\frac{l+1}{2l+1}}Y_{l1}\end{pmatrix}$$

и разложим по ним $Y_{l0}\begin{pmatrix}1\\0\end{pmatrix}$:

$$Y_{l0}\begin{pmatrix}1\\0\end{pmatrix}=\frac{1}{\sqrt{2l+1}}\left(\sqrt{l+1}Y_l^+ + \sqrt{l}Y_l^-\right).$$

Подставляя (3) в (1), получаем:

$$\bigcup = \frac{2\sqrt{\pi}}{kr}\sum_{l=0}^{\infty}\sum_I il\left(\sqrt{l+1}Y_l^+ + \sqrt{l}Y_l\right)\times$$
$$X\sin\left(kr-\frac{\pi l}{2}\right)C_z^{It}z\Phi_z^I =$$
$$= \frac{\sqrt{\pi}}{lkr}\sum_{l=0}^{\infty}\sum_I\left(\sqrt{l+1}Y_l^+ + \sqrt{l}Y_l\right)\times$$
$$XC_I^{I\tau}z\Phi_z^I\left(e^{ikr}-(-1)^l e^{-ikr}\right) =$$
$$= \frac{\sqrt{\pi}}{ik}\sum_{l=0}^{\infty}\sum_I C_I^{I\tau}z\Phi_z^I\left(\sqrt{l+1}Y_l^+ + \sqrt{l}Y_l^-\right)\frac{e^{ikr}}{r}-$$
$$-\frac{\sqrt{\pi}}{ik}\sum_{l=0}^{\infty}\sum_I C_I^{I\tau}z\Phi_I^I\left(\sqrt{l+1}Y_l^+ + \sqrt{l}Y_l\right)\times$$

23

1+22

Воспользуемся разложением падающей волны по собственным функциям сохраняющихся операторов (см. формулу (4) предыдущей задачи).

Каждый член этой суммы, соответствующий определенным значениям (l, J, I), будет рассеиваться независимо от других.

Следовательно, число частиц, обладающих (l, J, I), в процессе упругого рассеяния не меняется, поэтому влияние рассеивающего центра сводится к умножению на некоторый фазовый множитель $e^{2i\delta_{l\pm}^I}$. Здесь $\delta_{l\pm}^I = \delta_{l,J=1\pm\frac{1}{2}}^I$ зависит от l, J, I и не зависит от I_z вследствие гипотезы об изотопической инвариантности.

Следует заметить, что рассеивающий центр не влияет на сходящиеся волны, а влияет только на расходящиеся. Тогда волновая функция системы с учетом рассеяния запишется

$$\times(\quad -1)^l\frac{e^{-ikr}}{r}.$$

В ВиДе

$$\psi = \frac{\sqrt{\pi}}{lk}\sum_I\sum_{l=0}^{\infty}C_{I_z}^{I_z}z\times$$
$$\times\Phi_{I_z}^I\left(\sqrt{l+1}Y_l^+e^{2ii_l^l} + \sqrt{l}Y_l e^{2ii_{l-}^I}\right)\frac{e^{ikr}}{r}-$$
$$-\frac{\sqrt{\pi}}{ik}\sum_I\sum_{l=0}^{\infty}C_{I_z}^{I\tau}\Phi_I^I\left(\sqrt{l+1}Y_l^+ + \sqrt{l}Y_l^-\right)\frac{e^{-lkr}}{r}.$$

На больших расстояниях от рассеивающего центра ее можно представить в виде

$$\dot{\varphi} = \bigcup_{\text{пад}} + f\frac{e^{ikr}}{r}.$$

Здесь f-амплитуда рассеяния. Отсюда, вычитая из (1) выражение для (???)тал (см. формулу (4) задачи 22 § 9), получим:

$$f = \frac{\sqrt{\pi}}{ik}\sum_I\sum_{l=0}^{\infty}C_{I_z}^{I_z z}\times$$
$$\times\Phi_{I_z}^I\left\{\sqrt{l+1}Y_l^+\left(e^{2ii_{l+}^I}-1\right)+\sqrt{l}Y_l^-\left(e^{2ii_l^I}-1\right)\right\}.$$

Ф Фукций $\Phi_{I_z}^I$ разложим по собственным функциям оператора I_z

$$\Phi^I_{I_z} = C^{I_z}_{z}\delta(\pi - \pi_i)\delta(n-\tau_z) + C^{I_z - \tau_z}_{I_z}\delta(\pi-\pi_k)\delta(n+\tau_z),$$

где коэффициенты Клебша - Жордана $C_{I_z^I \tau_z}$ определяются из таблицы (2) задачи 22, а $\pi_k = \pi_i + 2\tau_z$. Подставляя (3) в (2), получим:

$$f = \frac{\sqrt{\pi}}{ik}\sum_I \sum_{l=0}^{\infty}\left\{G^{I\tau_z}_{I_z z_z}\delta(\pi-\pi_i)\,\hat{\delta}(n-\tau_z) + G^{I_{\bar{h}}}_{I_{z'}-\tau_z}\delta(\pi-\pi_k)\,\delta(n+\tau_z)\right\}\times$$
$$\times\left\{\sqrt{l+1}Y_l^+\left(e^{2ii^I_{l+}}-1\right)+\sqrt{l}Y_l^-\left(e^{2ii^I_{l-}}-1\right)\right\},$$

где

$$O^{I\tau_z}_{I_z\tau_z} = C^{I\tau_z}_z C^{I\tau'_z}_{I_z}$$

и z'_z обозначает конечное состояние нукпона.
Тогда, полагая:

$$f = f^{\tau_z}_{\tau_z}\hat{0}(\pi-\pi_i)\,\delta(n+\tau_z) +$$
$$-1 - f^{\tau}_z\delta(\pi-\pi_k)\,\delta(n+\tau_z)$$

Получим:

$$f^{\tau_z}_z = \frac{\sqrt{\pi}}{ik}\sum_I\sum_{i=0}^{\infty}C^{I\tau_z}_{z_z},\sqrt{l+1Y_l^+}\left(e^{2i\delta^I_l}+(1)+1\right.$$
$$\left.+\sqrt{lY_l-\left(e^{2i\delta^I_l}-1\right)}\right\}$$

где $G^{I\tau_z}_z$ для требуемых в задаче реакций даны в следующей таблице:

Реакция	$p^+ \to p^+$	$p^- \to p^-$	$p^- \to n^0$
$G^{3/2\,\tau_z}_{I_z\tau_z}$	1	$\frac{1}{3}$	$\frac{\sqrt{2}}{3}$
$G^{1/2\,\tau_z}_{I_z\tau_z}$	0	$\frac{2}{3}$	$-\frac{\sqrt{2}}{3}$

Подставляя эти значения $G^{It_z}_{I_z;}$ в (4), окончательно получаем:

$$f(p^+,p^+) = \frac{\sqrt{\pi}}{lk}\sum_{l=0}^{\infty}\left\{\sqrt{l+1}Y_l^+\left(e^{2ii_l^{8/2}}-1\right)+\right.$$
$$\left.+\sqrt{l}Y_l-\left(e^{2i\delta^2/2}-1\right)\right\},$$
$$f(p^-,p^-) = \frac{\sqrt{\pi}}{3ik}\sum_{i=0}^{\infty}\left\{\sqrt{l+1}Y_l^+\left(e^{2ii_l^2/2}+2e^{2ii^2/2}+3\right)+\right.$$

24

1+23

Таблица коэффициентов $G^{I_z}_{r_z\tau'_z}$ для все возможных реакций мезонов с нуклонами имеет вид

№ п/п	Реакция	I_z	$G^{3/2\,\tau_z}_{I_z\tau_z}$	$G^{1/2\,\tau_z}_{I_z\tau_z}$
1	$p^+ \to p^+$	3/2	1	0
2	$p^0 \to p^0$	1/2	2/3	1/3
3	$p^0 \to n^+$	1/2	$\sqrt{2}/3$	$-\sqrt{2}/3$
4	$p^- \to n^0$	$-1/2$	$\sqrt{2}/3$	$-\sqrt{2}/3$
5	$p^- \to p^-$	$-1/2$	1/3	2/3
6	$n^+ \to n^+$	1/2	1/3	2/3
7	$n^0 \to p^-$	$-1/2$	$\sqrt{2}/3$	$-\sqrt{2}/3$
8	$n^+ \to p^0$	1/2	$\sqrt{2}/3$	$-\sqrt{2}/3$
9	$n^0 \to n^0$	$-1/2$	2/3	1/3
10	$n^- \to n^-$	$-3/2$	1	0

$$f(p^-,\ n_0)=\frac{\sqrt{2\pi}}{3ik}\sum_{l=0}^{\infty}\Big[\sqrt{l+1}Y_l^+\left(e^{2i\delta_{l+}^{3/}}-e^{2i\delta_{l+}^{1/}}\right)+\sqrt{l}Y_l^-\left(e^{2i\delta_{l-}^{3/}}-e^{2i\delta_{l-}^{1/}}\right)\Big].$$

Так как фазы не зависят от I_z в силу гипотезы об изотопической инвариантности, то из таблицы (1) и формулы (4) задачи 23§9 непосредственно следует:
$f\left(p^+,p^+\right)=f\left(n^-,n^-\right)$,
$f\left(p^-,p^-\right)=f\left(n^{\div},n^+\right)$,
$f\left(p^0,n^+\right)=f\left(n^+,p^0\right)=f\left(p^-,n^0\right)=f\left(n^0,p^-\right)$,
$f\left(p^0,p^0\right)=f\left(n^0,n^0\right)$.
Выражения для первых трех амплитуд даны в задаче 23. Из таблицы (1) легко видеть, что

$$f\left(p^0,p^0\right)=\frac{1}{2}\left[f\left(p^+,p^+\right)+f\left(p^-,p^-\right)\right]$$

Пользуясь таблицей (1), получаем:
$f\left(p^+,p^+\right)=f\left(n^-,n^-\right)=f^{3/2}$
$f\left(p^-,p^-\right)=f\left(n+,^4n+\right)=\frac{1}{3}\left[f^3+2+2f^{i_i'}\right]$,
$f\left(p^0,n^+\right)=f\left(n^+,p^0\right)=$

$$=f\left(p^-,n^0\right)=f\left(n^0,p^-\right)=\frac{\sqrt{2}}{3}|f''...f^1!\Bigg]$$

1+3

$f\left(p^0,p^0\right)=f\left(n^0,n^0\right)=\frac{1}{3}\left[2f^{3/2}+f^{1/2}\right]$

1+24

Дифференциальное сечение рассеяния:

$$\frac{d\sigma}{d\Delta 2}=|f|^2,\ \text{где } dQ=\sin\theta d\theta d\varphi.$$

Полное сечение рассеяния:

$$\sigma=\int_0^{2\pi}\int_0^{\pi}|f|^2\sin\theta dtd\varphi_0.$$

Подставляя сюда амплитуды рассеяния указанных реакций, найденные в задаче 23 и учтя ортонормированность функций Паули

$$\iint\left(Y_l^+\right)^+\left(Y_{l'}^+\right)dQ=\iint\left(Y_l^-\right)^+\left(Y_{l'}^-\right)dQ=\delta l_{l'},$$
$$\iint\left(Y_l^+\right)^+\left(Y_{l'}^-\right)dQ=\iint\left(Y_l^-\right)^+\left(Y_{l'}^+\right)dQ=0,$$

получаем:

$$\sigma\left(p^+,p^+\right)=\frac{4\pi}{k^2}\sum_{l=0}^{\infty}\left\{(l+1)\sin^2\delta_{l+}^{3//+}+l\sin^2\delta_{l-}^{3/4}\right\},$$

$$\sigma\left(p^-,p^-\right)=\frac{4\pi}{3k^2}\sum_{l=0}^{\infty}\{(l+1)\times$$
$$\times\left[\sin^2\delta_{l+}^{8/2}+2\sin^2\delta_{l++}^{1/2}-\frac{2}{3}\sin^2\left(\delta_{l+}^{3/2}-\delta_{l+/2}^{1/2}\right)\right]+$$
$$+l\left[\sin^2\delta_{l-}^{3/2}+2\sin^2\delta_{l-}^{1/2}-\frac{2}{3}\sin^2\left(\delta_{l-}^{8/2}-\delta_{l-}^{1/2}\right)\right]\Bigg\},$$

$$\sigma\left(p^-,n^0\right)=\frac{8\pi}{9k^2}\sum_{l=0}^{\infty}\left\{(l+1)\sin^2\left(\delta_{l+}^{8/2}-\delta_{l+}^{1/2}\right)+l\sin^2\left(\delta_{l+}^{8/2}-\delta_{l-}^{1/2}\right)\right\}.$$

1+25

Дадим подробное решение для реакции (p^+, p^+). Амплитуда рассеяния для S - и P-волн имеет вид (см. задачу 23§9):

$$f\left(p^+, p^+\right) = \frac{\sqrt{\pi}}{lk}\left\{\alpha_0 Y_0^+ + \sqrt{2}\alpha_1 Y_1^+ + \beta_1 Y_1^-\right\},$$

rge

$$\alpha_0 = e^{2i\delta_0^{8/2}} - 1; \quad \alpha_1 = e^{2i\delta_1^{8}/\frac{2}{+}} - 1; \quad \beta_1 = e^{2ii_1^{2/2}-} - 1.$$

Тогда дифференциальное сечение рассеяния для S - и P-волн равно (здесь учтены явные выражения для функций Паули (см. задачу 22§9))

$$\begin{aligned}
&\frac{k^2}{\pi}\frac{d\sigma}{d\underline{Q}} = |Y_{00}|^2|\alpha_0|^2 + \\
&+ \frac{1}{\sqrt{3}}|Y_{00}||Y_{10}|\left\{2\left(\alpha_0\alpha_1^* + \alpha_0^*\alpha_1\right) + \left(a_0, 3_1^* + \alpha_{0,\beta_1}^*\right)\right\} + \\
&+ \frac{1}{3}|Y_{10}|^2\left\{4|\alpha_1|^2 + |3_1|^2 + 2\left(\alpha_1\beta_1^* + \alpha_1^*\beta_1\right)\right\} + \\
&+ \frac{2}{3}|Y_{11}|^2\left\{|\alpha_1|^2 + |\beta_1|^2 - \left(\alpha_1\beta_1^* + \alpha_1^*\beta_1\right)\right\}.
\end{aligned}$$

Так как шаровые функции Y_{lm} равны

$$Y_{00} = \frac{1}{\sqrt{4\pi}}; \quad Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta; \quad Y_{11} = \sqrt{\frac{3}{8\pi}}\sin\theta e^{i\varphi},$$

то дифференциальное сечение запишется в виде

$$k^2\frac{d\sigma}{d\theta} = A + B\cos\theta + C\cos^2\theta,$$

где коэффициенты A, B, C равны

$$\begin{aligned}
A &= \frac{1}{4}\left\{|\alpha_0|^2 + |\alpha_1|^2 + |\beta_1|^2 - \left(\alpha_1\beta_1^* + \alpha_1^*\beta_1\right)\right\}; \\
B &= \frac{1}{4}\left\{2\left(\alpha_0\alpha_1^* + \alpha_0^*\alpha_1\right) + \left(\alpha_{01}^* + \alpha_0^*\beta_1\right)\right\}; \\
C &= \frac{3}{4}\left\{|\alpha_1|^2 + \left(\alpha_1\beta_1^* + \alpha_1^*\beta_1\right)\right\}.
\end{aligned}$$

Чтобы выразить коэффициенты A, B, C через фазы, воспользуемся тождествами

$$\begin{aligned}
&|e^{2i\cdot x} - 1|^2 = 4\,\mathrm{sit}^2\, x; \\
&\left(e^{2ix} - 1\right)\left(e^{-2iy} - 1\right) + \left(e^{-2ix} - 1\right)\left(e^{2iy} - 1\right) = \\
&= 4\left[\sin^2 x + \sin^2 y - \sin^2(x - y)\right].
\end{aligned}$$

Тогда:

$$\left.\begin{aligned}
A\left(p^+, p^+\right) = &\quad \sin^2\delta_0^{3/2} + \sin^2\left(\delta_{1+}^{3/2} - \delta_1^{3/2}\right); \\
B\left(p^+, p^+\right) = &\quad 3\sin^2\delta_0^{33/2} + 2\sin^2\delta_{1+}^{3/2} + \sin^2\delta_1^{3/2} - \\
&\quad -2\sin^2\left(\delta_0^{3/2} - \delta_{1+}^{3/2}\right) - \sin^2\left(\delta_0^{3/2} - \delta_{1-}^{3/2}\right); \\
C\left(p^+, p^+\right) = &\quad 3\left\{2\sin^2\delta_{1+}^{3/4} + \sin^2\delta_{1-}^{3/2} - \sin^2\left(\delta_{1+}^{8/2} - \delta_{1-}^{3/2}\right)\right\}.
\end{aligned}\right\}$$

Указанным способом легко подсчитать коэффициенты A, B, C для реакций (p^-, p^-)и $\left(p^-, n^0\right)$. Приведем лишь окончательные результаты:

$$\begin{aligned}
A\left(p^-\ p^-\right) = &\frac{1}{3}\sin^2\delta_0^{2/2} + \frac{2}{3}\sin^2\delta_0^{1/2} - \frac{2}{9}\sin^2\left(\delta_0^{3/2} - \delta_0^{1/2}\right) + \\
&+ \frac{1}{9}\sin^2\left(\delta_{1+}^{3/2} - \delta_{1-}^{3/2}\right) - \frac{2}{9}\sin^2\left(\delta_{1-}^{3/2} - \delta_{1-}^{1/2}\right) + \\
&+ \frac{2}{9}\sin^2\left(\delta_{1-}^{3/2} - \delta_{1+}^{1/2}\right) + \frac{2}{9}\sin^2\left(\delta_{1+}^{3/2} - \delta_1^{1/2}\right) + \\
&+ \frac{4}{9}\sin^2\left(\delta_{1-}^{1/2} - \delta_{1+}^{1/2}\right) - \frac{2}{9}\sin^2\left(\delta_{1+}^{3/4} - \delta_{1+}^{1/2}\right)
\end{aligned}$$

$$B\left(p^-,p^-\right)=\sin^2\delta_0^{3/2}+2\sin^2\delta_0^{1/2}+\frac{2}{3}\sin^2\delta_{1+}^{s/2}+$$
$$+\frac{4}{3}\sin^2\delta_{1+}^{2/s}+\frac{1}{3}\sin^2\delta_{1-}^{3/2}+\frac{2}{3}\sin^2\delta_{1-}^{1/2}-\frac{2}{9}\sin^2\left(\delta_0^{8/2}-\delta_{1+}^{3/2}\right)-$$
$$-\frac{4}{9}\sin^2\left(\delta_0^{3/3}-\delta_1^3/2\right)-\frac{1}{9}\sin^2\left(\delta_0^{3/2}-\delta_{1-}^{8/4}\right)-$$
$$-\frac{2}{9}\sin^2\left(\delta_0^{3/2}-\delta_1^{1/2}\right)-\frac{4}{9}\sin^2\left(\delta_0^{1/2}-\delta_{1+}^{2/2}\right)-\frac{8}{9}\sin^2\left(\delta_0^{1/2}-\delta_{1+}^{1/2}\right)-$$
$$-\frac{2}{9}\sin^2\left(\delta_0^{1/2}-\delta_1^{3/3}\right)-\frac{4}{9}\sin^2\left(\delta_0^{7/2}-\delta_1^{2/2}\right);$$

$$C\left(p^-,p^-\right)=2\sin^2\delta_{1+}^{3/2}+4\sin^2\delta_{1+}^{1/2}+\sin^2\delta_{1-}^{3/2}+\qquad+2\sin^2\delta_{1-}^{1/2}-\frac{2}{3}\sin^2\left(\delta_{1-+}^{2//}-\delta_{1+}^{1/2}\right)-$$
$$-\frac{1}{3}\sin^2\left(\delta_{1+}^{3/4}-\delta_{1-}^{3/2}\right)-\frac{2}{3}\sin^2\left(\delta_{1+}^2/\frac{2}{-2}\delta_{1-}^{1/2}\right)-$$
$$-\frac{2}{3}\sin^2\left(\delta_{1+}^{3/2}-\delta_{1-}^{3/2}\right)-\frac{2}{3}\sin^2\left(\delta_{1+}^{1/2}-\delta_{1-}^{3/2}\right);$$
$$A\left(p^-,n^0\right)=\frac{2}{9}\left\{\sin^2\left(\delta_0^{3/2}-\delta_0^{1/2}\right)+\sin^2\left(\delta_{1+}^{3/2}-\delta_{1+}^{1/2}\right)+\right.$$
$$+\sin^2\left(\delta_{1+}^{3/2}-\delta_{1-}^{3/2}\right)-\sin^2\left(\delta_{1+}^{3/2}-\delta_1^{2/2}\right).$$
$$-\sin^2\left(\delta_{1+}^{1/2}-\delta_{1-}^{2/2}\right)+\sin^2\left(\delta_{1+}^{1/2}-\delta_{1-}^{1/2}\right)+$$
$$\left.+\sin^2\left(\delta_1^{3/2}-\delta_{1-}^{1/2}\right)\right\};$$

$$B\left(p^-,n^0\right)=\frac{2}{9}\left\{-2\sin^2\left(\delta_0^{8/2}-\delta_{1+}^{3/2}\right)+2\sin^2\left(\delta_0^{3/2}-\delta_{+_+}^{1/2}\right)-\right.$$
$$-\sin^2\left(\delta_0^{s/4}-\delta_{1-}^{3/9}\right)+\sin^2\left(\delta_0^{8/3}-\delta_1^{1/2}\right)+$$
$$+2\sin^2\left(\delta_0^{1/2}-\delta_{1+}^{8/4}\right)-2\sin^2\left(\delta_0^{1/2}-\delta_{1+}^{1/2}\right)+$$
$$\left.+\sin^2\left(\delta_0^{1/2}-\delta_1^{3/2}\right)-\sin^2\left(\delta_0^{1/2}-\delta_1^{1/2}\right)\right\};$$
$$C\left(p^-,n^0\right)=\frac{2}{3}\left\{\sin^2\left(\delta_{1+}^{2/2}-\delta_{1+}^{z_1^{2/2}}\right)+\sin^2\left(\delta_{1+}^{8/2}-\delta_{1-}^{1/2}\right)-\right.$$
$$\left.-\sin^2\left(\delta_{1+}^{2/2}-\delta_{1-}^{3/2}\right)+\sin^2\left(\delta_{1+}^{2/2}-\delta_{1-}^{2/2}\right)-\sin^2\left(\delta_{1+}^{2/2}-\delta_{1-}^{1/2}\right)\right\}.$$

Полученные результаты имеют большое значение при изучении углового распределения рассеяния π-мезонов на протонах. Экспериментально можно проверить формулу (1) и определить коэффициенты A, B, C для реакций (p^+,p^+), (p^-,p^-), $\left(p^-,n^0\right)$. Тогда шесть неизвестных фаз $\delta_0^{3/2}, \delta_3^{1/2}, \delta_{1-1}^{2/3}, \delta_{1-}^{3/2}, \delta_{1+}^{1/9}, \delta_{1-}^{1/2}$ определяются из девяти уравнений (2), (3), (4), которые оказываются совместными.

Однако вычисленные фазы обладают неоднозначностью двоякого рода: во-первых, вследствие того, что в уравнения (2), (3), (4) входят квадраты синусов фаз и разностей фаз, последние определяются с точностью до знака; во-вторых, имеется несколько различных наборов фаз, удовлетворяющих опытным данным. Из них лучше других согласуется с экспериментом решение Ферми, в котором наибольший вклад в рассеяние вносит фаза $\delta_{1-1}^{3/,}$, проходящая через 90° при энергии мезона $E\approx 195$ Мэв в лабораторной системе координат, а фазы $\delta_{1-}^{3/3}, \delta_{1+}^{1/2}, \delta_{1-}^{1/2}$ малы.

Имеется ряд дополнительных критериев, позволяющих устранить указанные неоднозначности. Знаки фаз можно определить из соображений, основывающихся на принципе причинности, а также из опытов, специально учитывающих кулоновское взаимодействие. В выборе правильного решения могли бы помочь опыты по поляризации нуклонов отдачи, но в настоящее время они еще не поставлены. Ожидаемые величины поляризаций для реакций (p^+,p^+), (p^-,p^-), $\left(p^-,n^0\right)$ определяются в следующей задаче.

1+26

Рассмотрим подробно реакцию (p^+,p^+). Пусть спиновые функции протона:

$$\alpha=\begin{pmatrix}1\\0\end{pmatrix}\text{ для }\quad s_z=1/2;$$
$$\beta=\begin{pmatrix}0\\1\end{pmatrix}\text{ для }\quad s_z=-1/2.$$

Если вначале протон имел $s_z = 1/2$, то амплитуда рассеяния запишется в виде

$$f_{t_{i/2}} = f_{\alpha u}\alpha + f_{\alpha\beta,3}$$

и если вначале $\varsigma_z = -1/2$, то амплитуда рассеяния

$$f_{-1/2} = f_{\beta\alpha\alpha}\alpha + f_{\beta\beta\beta}3.$$

Здесь $f_{\alpha a}, f_{\beta\beta}$ - амплитуды рассеяния без переориентации спина и $f_{\alpha\beta}, f_{\beta\alpha}$ - с переориентацией спина. Амплитуды $f_{\alpha\alpha}$ и $f_{\alpha\beta}$ определяются из формул (5) задачи 23§9 как коэффициенты при столбцах $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ и $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, причем берутся только S и P-волны

$$f_{o\alpha} = \frac{\sqrt{\pi}}{tk}\left\{\alpha_0 Y_{00} + \frac{1}{\sqrt{3}}\left[2\alpha_1 + \beta_1\right]Y_{10}\right\},$$
$$f_{\theta\beta} = \frac{\sqrt{\pi}}{ik}\sqrt{\frac{2}{3}}\left(\beta_1 - \alpha_1\right)Y_{11},$$

где $\alpha_0, \alpha_1, \beta_1$ даны в задаче 26§9. Пользуясь выражениями для функций Паули при $m_j = 1/2$, легко получить:

$$f_{\beta\alpha} = \frac{\sqrt{\pi}}{ik}\sqrt{\frac{2}{3}}\left(\alpha_1 - \beta_1\right)Y_{1,-1};$$
$$f_{\beta\beta} = f_{\alpha\alpha}.$$

Если считать, что π-мезоны рассеиваются в плоскости xz, то полярный угол $\varphi = 0$, и следовательно:

$$f_{\alpha,3} = -f_{\beta\alpha}.$$

Тогда амплитуда рассеяния на протоне с $s_z = -1/2$ (см. (2))

$$f_{-1/2} = -f_{\beta\alpha}\alpha + f_{\alpha a i}3.$$

Так как вначале протоны не были поляризованы, то из формул (1) и (5) слелует, что и после рассеяния они останутся неполяризованными вдоль оси z.

Можно показать, что после рассеянииия поляризация протонов в плоскости xz отсутствует. Действительно, спиновые функции протона γ_θ и δ_0, соответствующие проекциям спина $1/2$ и $-1/2$ на ось z', проведенную в плоскости xz под углом θ к оси z, имеют вид

$$\begin{pmatrix} \gamma_\theta \\ \delta_\theta \end{pmatrix} = e^{-i\hat{y}_y\theta}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

(см. задачу 19§4), Тогда

$$\begin{aligned} f_{1/2} =& f_{\alpha\alpha}\alpha + f_{\alpha\beta}\beta = \\ &= \left(f_{\alpha\alpha}\cos\frac{\theta}{2} - f_{\alpha\beta}\sin\frac{\theta}{2}\right)\gamma_\theta + \left(f_{\alpha\alpha}\sin\frac{\theta}{2} + f_{z\beta}\cos\frac{\theta}{2}\right)\delta_0; \\ f_{-1/2} =& -f_{\sigma\beta}\alpha + f_{\alpha\alpha}\beta = \\ &= -\left(f_{\alpha\alpha}\sin\frac{\theta}{2} + f_{\sigma\beta}\cos\frac{\theta}{2}\right)\gamma_\theta + \left(f_{\alpha\alpha}\cos\frac{\theta}{2} - f_{\alpha\beta}\sin\frac{\theta}{2}\right)\delta_0, \end{aligned}$$

т. е. поляризации в любом направлении в плоскости xz нет.

Однако протоны будут поляризованы вдоль оси y, перпендикулярной плоскости рассеяния. Чтобы найти величину поляризации, выразим $f_{1/2}$ и $f_{-1/2}$ через спиновые собственные функции

$$\gamma = \frac{\alpha + i\beta}{\sqrt{2}}; \quad \delta = \frac{\alpha - i\beta}{\sqrt{2}},$$

соответствующие направлению спина вдоль и против оси y. Тогда

$$f_{1/2} = \frac{1}{\sqrt{2}}\left(f_{\alpha\alpha} - if_{\alpha\beta}\right)\gamma + \frac{1}{\sqrt{2}}\left(f_{\alpha\alpha} + if_{\alpha\beta}\right)\delta,$$
$$f_{-1/2} = \frac{-i}{\sqrt{2}}\left(f_{\alpha\alpha} - if_{\alpha\beta}\right)\gamma + \frac{i}{\sqrt{2}}\left(f_{\alpha\alpha} + if_{\alpha\beta}\right)\delta.$$

Отсюда получаем:

$$W_+ \sim |f_{\alpha\alpha} - if_{\alpha\beta}|^2; \quad W_- \sim |f_{\alpha 2} + if_{\alpha\beta}|^2,$$

где W_+и W_-−вероятности того, чго спин после рассеяния будет направлен соответственно параллельно или антипараллельно оси y. Заметим, что формулы (6) справедливы независимо от первоначального значения s_z протона. Подставляя в (6) выражения (3) и (4) для $f_{\alpha\alpha}$ и $f_{\alpha,3}$, получим:

$$W_\pm \sim |\alpha_0 + (2\alpha_1 + \beta_1)\cos\theta \mp i\,(\beta_1 - \alpha_1)\sin\theta|_1^2,$$

или

$$W_\pm \sim |\left(e^{2ii_0^{3/2}} - 1\right) + \left(2e^{2ii_1^{3/2}+-3} + e^{2ii_1^{3/2}}\right)\cos\theta\pm$$
$$\pm i\left(e^{2i\hbar_1^{3/2}+} - e^{2ii_1^{3/2}}\right)\sin\theta|^3.$$

Iодобным же образом получим для реакций (p^-, p^-)и $\left(p^-, n^0\right)$:

$$W_\pm\left(p^-, p^-\right) \sim |\left(e^{2i\delta_0^{3/2}} - 3 + 2e^{2i\delta_0^{1/2}}\right) +$$
$$+\left(2e^{2i\delta_1^{3/2}} - 9 + 4e^{2ii_1^{1/2}} + +e^{2i\delta_1^{8/2}} + 2e^{2ii_1^{1/2}}\right)\cos\theta\pm$$
$$\pm\, i\left(e^{2i\delta_1^{3/2}} + 2e^{2ii_1^{1/2}+} - e^{2i\delta_1^{3/s}} - 2e^{2i\delta_i^{1/2}}\right)\cos\theta\Big|^2$$
$$W_\pm\left(p^-, n^0\right) \sim |\left(e^{2i\hbar_0^{3/2}} - e^{2i6^1\dot{0}'^2}\right) +$$
$$+\left(2e^{2i\delta_{11}^{32}} + -2e^{2i\delta_1^{1/2}} + e^{2i\delta_1^{3/3}} - -e^{2i\delta_1^{1/2}}\right)\cos\theta+$$
$$\pm\, i\left(e^{2i\delta_1^{3/2}} + e^{2i\delta_1^{1/2}} + -e^{2i\delta_1^{3/2}} + e^{2i\hat{\delta}_1^{1/2}}\right)\sin\theta|^2.$$

18.1.15 General problems about of uncertainty and matter waves 1

(maybe I'll move all it to the .tex file before, but currently they are not so important, so they are here)

О3.1-2.1 Волны размером протона

При каких кинетических энергиях электрона и протона их длины волн де Бройля близки к размеру протона $r_\text{p} \approx 0,8 \cdot 10^{-13}$см.

Solution

(?? просто сравнить формулы нужно?)
2.1. $T_\text{p} \approx 880$МэВ; $T_\text{e} \approx pc \approx 1550$МэВ.

О3.1-2.2;Иродов-6.57. Дебройлевская и комптоновская волны

Определить кинетическую энергию T электрона, при которой его дебройлевская и комптоновская длины волн равны между собой.

Solution

Просто сравниваем величины и пользуемся законами релятивистской механики. Мы помним, что $\lambda = \frac{h}{p}$ $\lambda_c = \frac{h}{m_e c}$ По условию $p = m_e c$, поэтому из $p^2c^2 = E^2 - \left(mc^2\right)^2$, деля на m^2c^4 и добавляя единицу, имеем $2 = \left(\frac{E_k}{m_e c^2} + 1\right)^2$. В итоге

$$E_k = (\sqrt{2} - 1)m_e c^2$$

$T = mc^2(\sqrt{2} - 1) = 0,212$МэВ

О3.1-2.3 Рассеяние протона

Протон с дебройлевской длиной волны $\lambda = 0,001$ нм упруго рассеялся под углом $\pi/2$ на первоначально покоившейся α-частице. Определить дебройлевскую длину волны λ' рассеянного протона.

Solution

(? по идее ф Комтона сразу дает ответ. но в ответах какой-то другой метод, его пока не понял, ответ какой-то с корнем, вообще пока нет идей, откуда это???)

2.3. $\lambda' = \sqrt{5/3}\lambda = 0,00129$НМ.

О3.1-2.4 Масса фотона

В опытах по распространению радиоволн с длиной волны $\lambda = 300$ м было установлено, что скорость v их распространения в вакууме совпадает со скоростью света c с точностью до $0,05\%$. Оценить на основе этих результатов верхнюю границу массы фотона.

Solution

Допустим, что фотон имеет энергию покоя $m_\gamma c^2$, тогда

$$\mathscr{E} = \sqrt{p^2c^2 + m_\gamma^2 c^4}$$

$$u = \frac{d\mathscr{E}}{d\rho} = \frac{pc}{\sqrt{p^2 + m_\gamma^2 c^2}} = \frac{c}{\sqrt{1 + (m_\gamma c\lambda/h)^2}}; \qquad \frac{u}{c} = \left[1 + \left(\frac{m_\gamma c\lambda}{h}\right)^2\right]^{-1/2} \geqslant 1 - \delta.$$

Тут $\lambda = h/p$ - дебройлевская длина волны фотона. Заметим что скорость фотона, в вакууме зависит от длины волны λ, т. е. в этом случае должна наблюдаться дисперсия электромагнитных волн в вакууме. По условию задачи $\delta = 5 \cdot 10^{-4}$, поэтому $m_\gamma \leqslant \frac{2h^2\delta}{c^2\lambda^2}$.

Ответ: $m_\gamma \leqslant 2 \cdot 10^{-43}$г; $\quad m_\gamma c^2 \leqslant 1,1 \cdot 10^{-10}$эВ.

О3.1-2.5 Ненулевая масса и расстояния

В опытах при измерении расстояния между Землей и Луной $\left(L = 3,8 \cdot 10^5\right)$ методом радиолокации оказалось, что результаты в оптическом и радиодиапазоне ($\lambda_1 = 20$см) не совпадают. Отличие в результатах измерений объяснялось попаданием излучения в разные точки лунной поверхности, которые могли отличаться по высоте на $\Delta L = \pm 100$ м. С другой стороны, этот результат можно интерпретировать как результат отражения фотона с ненулевой массой от ровной поверхности. Принимая это, оценить возможную верхнюю границу массы фотона m_γ (в эВ).

Solution

$$\mathscr{E} = \sqrt{p^2c^2 + m_\gamma^2 c^4}$$

$$u = \frac{d\mathscr{E}}{d\rho} = \frac{pc}{\sqrt{p^2 + m_\gamma^2 c^2}} = \frac{c}{\sqrt{1 + (m_\gamma c\lambda/h)^2}}; \qquad \frac{u}{c} = \left[1 + \left(\frac{m_\gamma c\lambda}{h}\right)^2\right]^{-1/2} \geqslant 1 - \delta.$$

$$m_\gamma \leqslant \frac{2h^2\delta}{c^2\lambda^2} = \frac{2hc}{\lambda_1}\sqrt{\frac{\Delta L}{L}} \approx 0,6 \cdot 10^{-8}\text{эВ}.$$

О3.1-2.6 Показатель преломления и работа выхода

Найти выражение для показателя преломления n электронных волн через работу выхода $A_0 = eV_0$ (V_0 - внутренний потенциал кристалла).

Solution

(??? я забыл начальные формулы фотоэффекта, тут длина волны через частоту выражается, а та почему через корень???? также, перепишу условие, там V нужно тоже задать)

$n = \frac{\lambda_0}{\lambda'} = \sqrt{\frac{\mathscr{E}+A_0}{\mathscr{E}}} = \sqrt{1 + \frac{V_0}{V}}$

$\mathscr{E}$ и V соответственно энергия электрона в вакууме и разность потенциалов, пройденная им).

О3.1-2.7 Закон преломления

Показать, что при преломлении электронной волны соблюдается закон преломления $\sin\varphi/\sin\varphi' = n$.
Указание. При проникновении в кристалл меняется лишь нормальная компонента скорости электрона.

Solution

(?? надо теорию перечитать)

О3.1-2.8 Модификация ф. Брэгга-Вульфа

Как нужно изменить формулу Брэгга-Вульфа, чтобы учесть преломление волн на поверхности кристалла? Считать, что отражающая плоскость параллельна поверхности кристалла.

Solution

(??? тоже пока это не понимаю. я условие не понял, мы изначально не учитываем что ли преломление?)
2.8. $2d\sqrt{n^2 - \cos^2\theta} = m\lambda_0$, где λ_0 - длина волны в вакууме, n - показатель преломления волн де Бройля, θ - угол скольжения.

О3.1-2.9 Показатель преломления электронных волн

Пучок электронов, ускоренный разностью потенциалов $V = 150$ В, падает на поверхность серебра, внутренний потенциал которого $V_0 = 15$ В. Найти показатель преломления электронных волн в серебре.

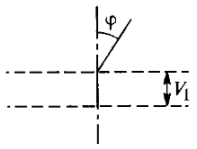
Solution

(??? как и в 2.6 не знаю, почему корень?)

$$n = \frac{\lambda_0}{\lambda'} = \sqrt{\frac{\mathscr{G} + A_0}{\mathscr{G}}} = \sqrt{1 + \frac{V_0}{V}} = 1,05$$

О3.1-2.10 Две сетки

Электроны с кинетической энергией $T = 100$ эВ падают под углом $\varphi = 30^\circ$ к нормали на систему, состоящую из двух параллельных сеток, между которыми создана разность потенциалов $V_1 = 36$ В:



Полагая, что потенциал нижней сетки выше, чем верхней, найти относительный показатель преломления n сред, расположенных по обе стороны от сеток. При какой разности потенциалов V_2 произойдет полное отражение электронов от второй сетки?

Solution

(???)
Очевидно, что полная энергия электрона, преодолевающего потенциальный барьер, сохраняется: $\mathscr{E} = T + U = \text{const}$, откуда $T = T_1 + eV_1$, где T и T_1 - кинетическая энергия до и после барьера. При этом

$$T = \frac{p^2}{2m} = \frac{p_\perp^2 + p_\parallel^2}{2m}$$

$p_\perp$ и $p_\parallel$- нормальная и касательная к границе раздела компоненты импульса. Поскольку скачок U связан с силами, действующими перпендикулярно к границе (электрического поля), то $p_\parallel$ =const. Откуда $p\sin\varphi = p_1\sin\varphi_1$. Относительным коэффициентом преломления сред является величина

$$n = \frac{\lambda}{\lambda_1} = \frac{h/p}{h/p_1} = \frac{p_1}{p} = \frac{\sin\varphi}{\sin\varphi_1} = \sqrt{\frac{T - eV_1}{T}} = \sqrt{1 + \frac{|e|V_1}{T}}.$$

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Полное отражение электронов произойдет, когда $\sin\varphi_1 = 1$ (при этом разность потенциалов равна V_2), т. е.

$$\sin\varphi_1 = \frac{\sin\varphi}{\sqrt{1 + (|e|V_2)/T}} = 1 \text{ или } \frac{1}{4} = 1 + \frac{|e|V_2}{T}$$

откуда и следует второй ответ.

Ответ: $n = \sqrt{\frac{T+|e|V_1}{T}} = 1,17; V_2 = -\frac{3}{4}\frac{T}{|e|} = -75$ В, где e - заряд электрона.

О3.1-2.11

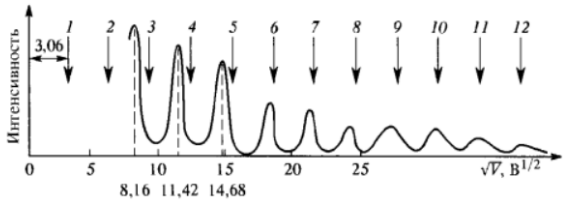
Пучок электронов падает перпендикулярно на поликристаллическую пластинку из хлористого натрия, постоянная решетки которого $a = 0,56$ нм. В результате брэгговского рассеяния пучка на фотопластинке Ф, расположенной на расстоянии $L = 25$см от пластинки , возникают концентрические дифракционные кольца (рис. 4). Определить энергию электронов, зная, что радиус первого кольша равен $R = 0.5$см.

2.

11. $\mathscr{E} = \frac{h^2}{2m}\left(\frac{L}{Ra}\right)^2 \approx 1,2 \cdot 10^4$ эВ.

О3.1-2.12 Опыт Дэвиссона и Джермера

На рис. ниже приведена кривая, полученная в опытах Дэвиссона и Джермера по рассеянию электронов от монокристалла никеля, падающих под углом скольжения 80°. По оси абсцисс отложено значение $\sqrt{V}$, где V - энергия электронов в вольтах, по оси ординат - относительная интенсивность рассеянных электронов. При больших порядках отражения m максимумы эквидистантны (расстояние между ними $3,06$ В$^{1/2}$), а при малых эта закономерность, показанная стрелками, нарушается. Оценить немонохроматичность используемых электронов и показатель преломления никеля для волны де Бройля электронов, соответствующих 3-му, 4-му и 5 -му максимумам, которые наблюдаются при $\sqrt{V}$, равном соответственно $8,16, 11,42$ и 14,68 В $^{1/2}$. Найти межплоскостное расстояние d никеля.



2.

12*: Решение. Для нерелятивистского электрона $\mathscr{E} = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} \propto \frac{1}{\lambda^2}$. Поэтому искомую немонохроматичность электронов $\Delta\mathscr{E}/\mathscr{E}$ легко оценить по числу наблюдаемых отражений $m_{\max} = 12$, откуда следует $\Delta\lambda = \frac{\lambda}{m_{\max}} \approx \frac{\lambda}{12}$. И далее $\left|\frac{\Delta\mathscr{E}}{\mathscr{E}}\right| = 2\left|\frac{\Delta\lambda}{\lambda}\right| = \frac{1}{6}$.

Вне металла скорость электрона $v_1 \propto \sqrt{V}$, внутри металла $v_2 \propto \propto \sqrt{V_0 + V}$, где V_0 - внутренний потенциал металла. Таким образом, показатель преломления металла

$$n = \frac{\boldsymbol{v}_2}{\boldsymbol{v}_1} = \sqrt{1 + \frac{V_0}{V}}$$

Эквидистантное расположение максимумов интенсивности отраженных электронов наблюдается, когда внутренний потенциал металла

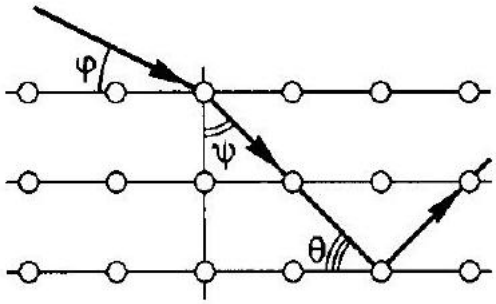


Рис. 138 $V_0 \ll V$. Это соответствует показателю преломления кристалла $n = 1$ (для $m \geqslant 6$). В этом случае в соответствии с формулой Брэгга-Вульфа (рис. 138)

$$2d\sin\varphi = m\lambda; \quad \lambda = \frac{2\pi\hbar}{\sqrt{2meV}}; \quad \sqrt{V} = \frac{2\pi\hbar}{\lambda\sqrt{2me}}$$

Последнее соотношение обычно записывают так

$$\sqrt{V} = \frac{12,26}{\lambda\,[\lambda]} = \frac{12,26m}{2d\sin\varphi}$$

где d следует подставлять в ангстремах [Å], а результат $\sqrt{V}$ получается в $\text{В}^{1/2}$. В нашем случае при $m = 1\sqrt{V} = 3,06\ \text{В}^{1/2}$, и поэтому межплоскостное расстояние $d = 2,03$Å. Из рис. 5 и условия задачи следует, что при $m < 6$ максимумы интенсивности неэквидистантны. Это означает, что при соответствующих энергиях показатель преломления отличается от 1 .

Закон преломления волн де Бройля идентичен классическому закону Снеллиуса:

$$\frac{\cos\varphi}{\sin\psi} = n; \cos\psi = \sqrt{1-\sin^2\psi} = \frac{1}{n}\sqrt{n^2-\cos^2\varphi}$$

По формуле Брэгга-Вульфа $n\cdot 2d\sin\theta = m\lambda$ или $n\cdot 2d\cos\psi = m\lambda$, откуда следует

$$2d\sqrt{n^2-\cos^2\varphi} = m\lambda$$

Обозначим через V' ускоряющий потенциал, соответствующий энергиям электронов, когда $n \neq 1$. Тогда

$$\sqrt{V'} = \frac{12,26}{\lambda[\text{Å}]} = \frac{12,26m}{2d\sqrt{n^2-\cos^2\varphi}}$$

Из соотношения $\sqrt{\frac{V}{V'}}$ мы и определим n : $\sqrt{\frac{V}{V'}} = \frac{\sqrt{n^2-\cos^2\varphi}}{\sin\varphi}$, откуда $n = \left(\frac{V}{V'}\sin^2\varphi + \cos^2\varphi\right)^{1/2}$.

Для $m = 5; \sqrt{V'} = 14,68\ \text{В}^{1/2}; \sqrt{V} = 15,3\ \text{В}^{1/2}; \quad n = 1,04.$
Для $m = 4; \sqrt{V'} = 11,42\ \text{В}^{1/2}; \sqrt{V} = 12,24\ \text{В}^{1/2}; n = 1,07.$
Для $m = 3; \sqrt{V'} = 8,16\ \text{В}^{1/2}; \sqrt{V} = 9,18\ \text{В}^{1/2}; \quad n = 1,12.$

О3.1-2.13 Падение электронов на движущейся кристалл

Параллельный пучок моноэнергетических нерелятивистских нейтронов, движущихся со скоростью v, падает на плоскую поверхность кристалла под углом скольжения θ_0 и испытывает на ней брэгговское отражение n-го порядка. Кристалл приводят в движение с постоянной скоростью u в направлении нормали к отражающей плоскости (рис. 6). Под каким углом θ к отражающей плоскости надо направить пучок таких же нейтронов, чтобы наблюдалось брэгговское отражение их от движущегося кристалла в прежнем порядке n? При какой скорости такое отражение возможно?

О3.1-2.15 Брэгговское отражение нейтронов

Чтобы получить пучок нейтронов, обладающих заданной энергией $\mathscr{E} = 1$ эВ, используют брэгговское отражение первого порядка от кристалла LiF, для которого расстояние между плоскостями кристаллической решетки $d = 2,32$Å. На кристалл падает пучок нейтронов с различными энергиями. 1) Оценить разброс нейтронов по энергиям $\Delta\mathscr{E}$ в отраженном пучке, если угловая ширина этого пучка $\Delta\varphi = 0,1^\circ$. 2) Какую толщину кристалла D следует выбирать в этом эксперименте? Кристалл вырезан так, что отражающие плоскости параллельны поверхности кристалла.

Solution

Условие Брэгга-Вульфа и масштаб бедствия по углам отклонения:

$$\sin\varphi = \frac{\lambda}{2d}$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} \approx 0.287\text{Å}; \sin\varphi \approx \varphi \approx 0.06$$

Из закономерности: $\lambda \sim \varphi \sim E^{-1/2}$:

$$\frac{\Delta\lambda}{\lambda} = \frac{\Delta\varphi}{\varphi} = \frac{\Delta E}{2E}$$

Выражаем отсюда $\Delta E = 2E\frac{\Delta\varphi}{\varphi} \approx 0.58$ эВ

Вопрос с толщиной. Дифракционная решетка с разрешающей способностью:

$$\frac{\Delta\lambda}{\lambda} \leq R = mN = 1 \cdot \frac{D}{d}$$

окончательно $D = \frac{\lambda}{2\Delta\varphi} = 82$Å

(!! подумаю про это еще раз)

О3.1-2.18

Один из способов монохроматизации медленных нейтронов состоит в следующем: в цилиндре радиусом $R = 10$ см и длиной $L = 1,0$ м делается винтовой паз шириной $b = 1$см с поворотом на угол $\varphi = 30°$ (рис. 10). Цилиндр вращается с частотой $n = 3000$ об/мин. Определить длину волны λ нейтронов, пропускаемых таким монохроматором, и оценить степень их монохроматизации $\Delta\lambda/\lambda$. Пучок нейтронов направлен вдоль оси цилиндра. Оценить оптимальную ширину паза, при которой достигается максимальная монохроматичность пучка.

О3.1-2.19 Брегговский интерферометр и предельный заряд нейтрона (!??!?)

Нейтроны со скоростью $v_0 = 5 \cdot 10^5$см/с падают на брэгговский интерферометр, состоящий из трех тонких монокристаллических пластинок, вырезанных перпендикулярно главным кристаллическим плоскостям. На каждой из пластинок волна де Бройля разделяется на прошедшую и отраженную (рис. 11). Результат интерференции фиксируется счетчиком нейтронов C, скорость счета которого зависит от разности фаз в плечах интерферометра. В од ном из плеч с помощью электродов (не показанных на рис. 11) на участке длиной $l = 1$ см создается электрическое поле с разностью потенциалов $V = 300$ В. Если бы у нейтрона был электрический заряд, то включение поля изменило бы скорость счета счетчика C. Найти, какой предельный заряд q нейтрона может быть обнаружен в таком опыте, если чувствительность интерферометра к сдвигу фаз составляет $\Delta\varphi = 0,1$ рад.

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О3.1-2.20

Нейтроны со скоростью $v_0 = 5 \cdot 10^5$см/ с падают на брэгговский интерферометр, описанный в задаче 2.19. В одном из плеч ин терферометра с помощью электродов (не показанных на рис. 11) на участке длиной $l = 1$ см создается электрическое поле $E = 3 \cdot 10^4$ В/cm. Если бы у нейтрона был электрический дипольный момент d, то включение поля повлияло бы на скорость счета счетчика. Найти, какая предельная величина d может быть обнаружена в таком опыте, если поле E параллельно предполагаемому направлению дипольного момента, а чувствительность интерферометра к сдвигу фаз $\Delta\varphi$ составляет 0,1 рад.

О3.1-2.21 Электроны проходят через лазер

Коллимированный пучок электронов с кинетической энергией $T = 1,65$ кэВ пропускается через резонатор лазера, работающего на длине волны $\lambda = 0,63$ мкм. При некоторых углах падения пучка относительно оси резонатора, близких к прямому, может наблюдаться брэгговское рассеяние электронов на стоячей электромагнитной волне (эффект Капицы-Дирака). Оценить возможные углы отклонения электронов.

Solution

(интересный эффект, в доп теории раздел про него создам, пока не совсем готов решать задачу)

О3.1-2.22

Исходя из требования, чтобы групповая скорость и волн де Бройля равнялась скорости движения v частицы, и пользуясь формулой Рэлея, связывающей фазовую и групповую скорости, определить фазовую скорость ш этих волн, а также найти связь между энергией частицы $\mathcal{E}$ и частотой v.

О3.1-2.23

Движение электрона описывается плоской монохроматической волной де Бройля. Электрон в таком состоянии обладает вполне определенным импульсом, но его координата совершенно не определена. Для определения x-координаты электрона на пути волны перпендикулярно к направлению ее распространения ставится непрозрачный экран со щелью. Пусть координатная плоскость XY расположена в плоскости экрана, причем ось X направлена перпендикулярно к щели. Показать, что в результате дифракции на щели возникает состояние электрона, в котором неопределённостей координаты электрона x и импульса p_x удовлетворяют соотношению Гейзенберга.

О3.1-2.24

В мысленном опыте Гейзенберга положение электрона определяется с помощью микроскопа при освещении электрона светом. Показать, что при таком методе измерения координата x и импульс p_x Электрона не могут быть определены более точно, чем требует соотношение неопределённостей Гейзенберга.

О3.1-2.25*

Скорость макроскопического тела измеряется по доплеровскому изменению частоты световой волны при отражении от этого тела (зеркала). Показать, что соответствующие неточности измерений импульса и положения тела удовлетворяют соотношению неопределённостей Гейзенберга.

О3.1-2.26

Какова должна быть кинетическая энергия T электронов (протонов) для исследования распределения заряда и ядерной материи внутри ядра с точностью $l \sim 1$ фм $\left(10^{-13}\text{см}\right)$, и структур с линейными размерами $l \sim 10^{-4}$ фм, что соответствует радиусу слабого взаимодействия?

О3.1-2.27

Из ускорителя через щель выводится короткий сгусток протонов с энергией $\mathcal{G} = 100$ кэВ. Оценить минимально достижимую ширину пучка протонов на расстоянии $L = 100$ м от выходной щели.

О3.1-2.28

Пучок протонов из ускорителя выводится через отверстие диаметром d. Используя соотношение неопределённостей, найти минимальный размер пучка на экране, расположенном на расстоянии $L = 1$ м от отверстия, если радиус орбиты в ускорителе $r = 10$ см, а величина магнитного поля в момент вывода $B = 300\Gamma c$.

О3.1-2.29

Оценить минимальный диаметр d пятна, создаваемого на экране пучком электронов, если время пролета от коллиматора до экрана равно 10^{-8}с.

О3.1-2.30

Оценить минимально достижимый диаметр d гятна, которое можно создать на детекторе пучком атомов серебра, испускаемых печью с температурой $t^\circ = 1200^\circ$с. Расстояние от выходной щели печи до детектора равно $L = 1$ м. Расчет произвести: 1) исхоая из волновой природы частиц (радиус первой зоны Френеля); 2) исходя из соотношения неопределённостей. Убедиться в эквивалентности обоих подходов.

О3.1-2.31 Радиус действия ядерных сил

Предполагая, что ядерные силы между нуклонами обусловлены обменом квантами ядерного поля - виртуальными пионами, оценить радиус Δr действия ядерных сил, если известно, что энергия покоя пионов $m_\pi c^2 \approx 140$ МэВ.

Solution

О3.1-2. 32

Оценить кинетическую энергию 8 электрона, локализованного в области пространства, радиус которого $r \sim 10^{-8}$см (атом) и $r \sim 10^{-12}$см (атомное ядро).

О3.1-2. 33

Оценить, при какой напряженности E электрического поля лазерного излучения может произойти пробой вакуума, т. е. разрыв виртуальных электрон-позитронных пар. См. также задачу 6.260 из второй части задачника.

О3.1-2.34 Минимальное видимое расстояние электронным микроскопом (??)

Определить теоретическое минимально разрешимое расстояние d электронным микроскопом при ускоряющем напряжении $V = 100$ кВ и числовой апертуре $A = 0,1$.

О3.1-2.35

Мезоатомы водорода (связанные состояния протона и мюона) исследуются с помощью электронного микроскопа с ускоряющим напряжением $V = 3$МВ. При какой числовой апертуре микроскопа можно определить размер мезоатома? Энергия покоя электрона $\oint_0 = 0,511$МВ, масса мюона $m_\mu \approx 200 m_\text{e}$.

О3.1-2.36

В новых сверхпроводящих материалах расстояние d между соседними атомами около 4Å. Определить, какую апертуру должен иметь электронный микроскоп с ускоряющим напряжением $V = 50$ кВ, чтобы можно было получить изображение кристаллической решетки этих материалов.

18.1.17 General problems about of uncertainty and matter waves 3

О3.1-2.37

У оптического микроскопа угловая апертура порядка 1, а у электронного она равна 10^{-4}. При каком напряжении, ускоряющем электроны, разрешающая сила этих приборов будет одинакова?

О3.1-2.38.

Электрон притягивается к поверхности жидкого гелия электростатическими силами изображения, гютенциальная энергия которых, как известно, равна

$$U(x) = \frac{e^2}{4x}\frac{\varepsilon - 1}{\varepsilon + 1}$$

где x - кратчайшее расстояние от электрона до поверхности, e - заряд электрона, $\varepsilon = 1,057$ - диэлектрическая проницаемость гелия (рис. 12). В то же время медленный электрон не может проникнуть внутрь гелия из-за отталкивания (так называемое отрицательное сродство гелия к электрону). Поэтому можно считать, что на поверхности ($x = 0$) потенциальная энергия испытывает бесконечный скачок и электрон оказывается в потенциальной яме (рис. 12, там просто типичный потенциал атома, падаем из бесконечности в нуле к минимуму, далее выпукло поднимаемся). Пользуясь этой моделью и соотношением неопределённостей, оценить по порядку величины среднее расстояние x электрона от поверхности гелия в основном состоянии и энергию связи $\mathscr{E}_\text{cs}$ Электрона вблизи поверхности гелия.

(дальше не выгружал, потому что их слишком много.)

О3.1-2.43. Оценки водорода и двухатомной молекулы

Оценить на основании соотношения неопределённостей радиус атома водорода в основном состоянии и энергию связи электрона в том же состоянии.

Определить на основании таких же оценок размер двухатомной молекулы и энергию её основного состояния,рассматривая молекулу как одномерный гармонический осциллятор с собственной частотой ω_0 и приведенной массой μ.

Solution. Атом водорода

(мб выше поставлю, хорошая по идее задача)
неопределённостей: $\Delta x \sim r; \Delta p \sim p \to p \cdot r = \hbar$. Полная энергия электрона в атоме водорода:

$$E = \frac{p^2}{2m} - \frac{e^2}{r} = \frac{\hbar^2}{2mr^2} - \frac{e^2}{r}$$

Атом находится в основном состоянии, значит, в состоянии с минимальной энергией. Найдем минимум через производную энергии по времени.

$$\frac{dE}{dt} = -\frac{\hbar^2 2r}{2mr^4} + \frac{e^2}{r^2} = 0 \to = \frac{\hbar^2}{me^2} = 0.53\text{Å}$$

Тогда энергия основного состояния:

$$E = \frac{\hbar^2}{2mr^2} - \frac{e^2}{r} = -\frac{me^4}{2\hbar^2} = -13.6 \text{ В}$$

Что интересно, эта оценка дает точно совпадающий с теорией Бора результат.

2. SOLUTIONS Волны де Бройля. Соотношение неопределенностей

2.

13. $\sin\theta = \sin\theta_0 \pm (u/v)$, где знак $\pm$ определяет направление движения кристалла ($/+$ - вниз, «-» - вверх). Отражение возможно при скоростях u, удовлетворяющих соотношению $|\sin\theta_0 \pm (u/v)| \leqslant 1$.

2.

14. $T = \frac{h^2}{3mk\lambda^2} = 14$ K, $d = \frac{\lambda}{2} = 0,335$.

2.

15: $D \geqslant \frac{\lambda}{2\Delta\varphi} = 82$Å.
Решение. Согласно условию Брэгга-Вульфа первый порядок ($m = 1$) отражения соответствуют углу

$$\sin\varphi = \frac{\lambda}{2d}$$

Длина волны, соответствующая энергии нейтрона Å $= 1$ эВ, равна $0,287$Å, поэтому $\lambda/(2d) \approx 0,06$. Это означает, что $\sin\varphi \approx \varphi \approx 0,06$. Очевидно, что $\frac{\Delta\varphi}{\varphi} = \frac{\Delta\lambda}{\lambda}$. Дебройлевская длина волны $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m\xi}} \propto \mathscr{E}^{-1/2}$. Поэтому $\left|\frac{\Delta\lambda}{\lambda}\right| = \frac{1}{2}\left|\frac{\Delta\mathscr{E}}{\varepsilon}\right|$. Откуда

$$\Delta\mathscr{E} = 2\mathscr{E}\frac{\Delta\lambda}{\lambda} = 2\mathscr{E}\frac{\Delta\varphi}{\varphi} \approx 0,58 \text{ эВ}$$

Толщину кристалла D выберем из тех соображений, что разрешающая способность такой системы $R = mN \geqslant \lambda/\Delta\lambda$, т. е. при $m = 1$ и числе интерферирующих пучков, равном числу слоев, $N = D/d$:

$$\frac{D}{d} \geqslant \frac{\lambda}{\Delta\lambda} = \frac{\varphi}{\Delta\varphi} = \frac{\lambda}{2d\Delta\varphi}$$

откуда

$$D \geqslant \frac{\lambda}{2\Delta\varphi} \approx 82\text{Å}.$$

Приведем другое решение этой задачи. Рассмотрим бесконечную решетку в направлении оси X (рис. 139). Волновая функция всей решетки представляет собой плоскую волну $A\exp\left(i\frac{p_x x}{\hbar}\right)$, где p_x - импульс решетки в направ-
лении оси X. При смещении всей решетки вдоль X на период d волновая функция умножается на $\exp\left(i\frac{p_x d}{\hbar}\right)$ и переходит сама в себя. Отсюда $p_x d = 2\pi m\hbar$, т. е. импульс, передаваемый решетке, квантован!

При

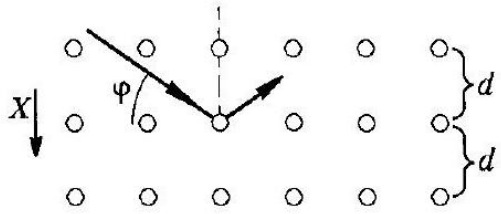


Рис. 139 упругом отражении $p_x = 2p\sin\varphi$, откуда следует $2d\sin\varphi = m(h/p) = m\lambda$. Таким образом, мы получили условие Брэг-га-Вульфа.

Если же решетка ограничена по x, то передаваемый по X решетке импульс приобретает неопределенность $\delta p_x \gtrsim h/D$. С другой стороны, $\delta p_x = 2p\delta(\sin\varphi) = 2p\cos\varphi\delta\varphi$. Поскольку $\cos\varphi \approx 1$, то

$$\delta\varphi = \frac{\delta p_x}{2p} \geqslant \frac{h}{D2p} \approx \frac{\lambda}{2D}.$$

Таким образом, искомая толщина кристалла $D \geqslant \frac{\lambda}{2\delta\varphi}$. Полагая $\delta\varphi \approx \Delta\varphi = 0,1°$, получим ответ.

2.

16: $T \approx \frac{\pi^2\hbar^2}{5kmd^2\theta^2} \approx 470$ K.

Решение. Под интенсивностью пучка молекул понимается плотность потока молекул с размерностью $\left[1/\left(\mathrm{cm}^2\cdot\mathrm{c}\right)\right]$. Плотность потока молекул, если считать их распределение по скоростям максвелловским, в интервале скоростей от v до $v + dv$ с точностью до известных констант равна

$$dj(v) \propto v\exp\left(-\frac{mv^2}{2kT}\right)v^2dv \qquad (*)$$

Далее пучок молекул испытывает рассеяние на кристаллических плоскостях LiCl. По условию Брэгта-Вульфа $2d\sin\theta = \lambda = 2\pi\hbar/(mv)$, где согласно графику порядок интерференции равен 1 , а m - масса молекулы водорода. Отсюда следует $v = \frac{\pi\hbar}{md\sin\theta}$. Из пучка шириной $d\theta$ дифракционное рассеяние испытывают молекулы из интервала скоростей dv, при этом

$$2d\cos\theta d\theta = -\frac{2\pi\hbar}{mv^2}dv$$

откуда $dv \propto v^2\cos\theta(v)d\theta$ с точностью до очевидных констант. Подставляя dv в (*), получим выражение для полного числа актов рассеяния молекул (плотность потока) в угол $d\theta$, имеющих скорость из заданного интервала скоростей, с точностью до известных констант

$$dN_{v,\theta} \propto v^3\exp\left(-\frac{mv^2}{2kT}\right)mv^2\cos\theta(v)d\theta.$$

Полагая, что $\cos\theta \approx 1$ (около 10°), $d\theta = \mathrm{const}$, найдем экстремум этой функции:

$$\frac{d}{dv}\left[v^5\exp\left(-\frac{mv^2}{2kT}\right)\right] = 0, \quad \text{откуда} \quad mv_{\max}^2 = 5kT$$

Таким образом,

$$T = \frac{m}{5k}\left(\frac{\pi\hbar}{md\sin\theta}\right)^2 \approx \frac{\pi^2\hbar^2}{5kmd^2\theta^2} \approx 470 \text{ K}.$$

При вычислениях из графика взято $\theta \approx 11°$.

2.

17. $\lambda = \frac{h\varphi}{m\Omega R} = 0,92$НМ, $\frac{\Delta\lambda}{\lambda} = \frac{a}{l\varphi} = 0,072$.

2.

18. $\frac{\hbar\varphi}{mLn} = 0,6$ нм; $\frac{\Delta\lambda}{\lambda} = \frac{b}{R\varphi} = 0,2$; $b_{\text{оптим}} = \sqrt{\lambda L} = 2,6 \cdot 10^{-3}$с (заметим, что этот численный ответ зависит от того, в какой форме взять соотношение неопределенностей: $\Delta p b \approx \hbar$ или h).

2.

19. $q < \frac{\Delta\varphi\hbar v_0}{Vl} \approx 5 \cdot 10^{-23}$ ед. СГСЭ.

2.

20* $d < \frac{\Delta\varphi\hbar v_0}{lE} \approx 5 \cdot 10^{-25}$ ед. СГСЭ или $d < e \cdot 10^{-15}$с, где e - заряд электрона в ед. СГСЭ.

Решение. Без поля сдвиг фаз на участке длиной l (разность хода!) $\varphi_0 2\pi l/h = lp_0/\hbar$, где p_0 - импульс частицы. При включенном поле импульс нейтрона должен измениться на Δp, и появится сдвиг фаз $\varphi_1 = l\left(p_0 + \Delta p\right)/\hbar$. Разность сдвигов фаз $\varphi_1 - \varphi_0 = \Delta\varphi = l\Delta p/\hbar$. Изменение импульса найдем из закона сохранения энергии: работа поля равна изменению кинетической энергии -

$$\frac{\left(p_0 + \Delta p\right)^2}{2m} - \frac{p_0^2}{2m} = Ed.$$

Из этого уравнения следует, что $\Delta p > Ed/v_0$. Отсюда получим $\Delta\varphi > \frac{l}{\hbar}\frac{Ed}{v_0}$ и дипольный момент $d < \frac{\Delta\varphi\hbar v_0}{lE}$.

2.

21*:

$$\theta \approx m\frac{2h}{\sqrt{2m_e T\lambda}} \approx m \cdot 10^{-4} \text{ рад, где } m = 1, 2, 3, \ldots$$

Решение. В резонаторе лазера устанавливается стоячая волна типа $E(x,t) \propto \sin kx e^{-i\omega t}$ (рис. 140). Электронная дебройлевская волна рассеивается на пучностях поля **E** стоячей волны, которые отстоят друг от друга на $\lambda/2$. Это и есть период структуры. От этих «плоскостей» происходит зеркаль ное отражение. Условие Брэгга-Вульфа (рис. 141) $2d\sin\varphi = m\lambda_{\text{дБ}}$;

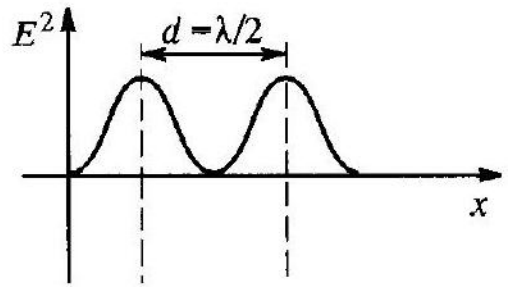


Рис. 140

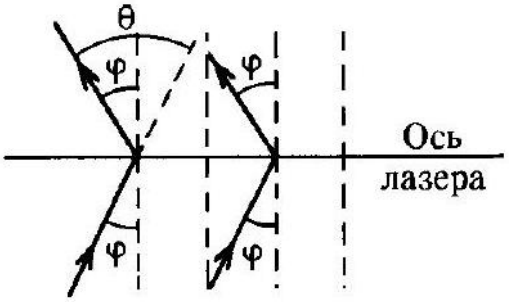


Рис. 141

$\lambda_{\text{дБ}} = h/p$. Поскольку кинетическая энергия электронов $T \ll m_e c^2$, то их можно считать нерелятивистскими. Поэтому $T = p^2/\left(2m_e\right)$ и $p = \sqrt{2m_e T}$. По условию угол скольжения $\varphi \ll 1$, таким образом,

$$\varphi \approx \dot{m}\frac{\lambda_{\text{ab}}}{2d} = m\frac{h}{\lambda\sqrt{2m_e T}}$$

Искомые углы отклонения

$$\theta = 2\varphi = m\frac{2h}{\lambda\sqrt{2m_e T}} \approx m \cdot 10^{-4} \text{ рад.}$$

2.

22*: $w = \frac{v}{2} + \frac{\text{const}}{v}, hv = \frac{1}{2}mv^2 + \text{const}$.

Решение. По формуле Рэлея групповая скорость $u = w - \lambda dw/d\lambda$. Полагая здесь $\lambda = h/p = h/(mv), u = v$ и рассматривая движение с нерелятивистскими скоростями, получим

$$v = w + v\frac{dw}{dv} = \frac{d}{dv}(wv),$$

откуда

$$w = \frac{v^2}{2} + \text{ const }, w = \frac{v}{2} + \frac{\text{const}}{v}.$$

Далее,

$$v = \frac{w}{\lambda} = \frac{v/2 + \text{ const }/v}{h/(mv)} = \frac{mv^2/2 + \text{ const}}{h}.$$

Во всех явлениях произвольные постоянные, входящие в выражения для v и w, не играют роли. Их можно положить равными нулю.

Разумеется, решение можно распространить и на движения с релятивистскими скоростями. Тогда, если отбросить не играющие роли постоянные интегрирования, формулы примут вид

$$w = \frac{c^2}{v}, hv = \frac{m_0 c^2}{\sqrt{1 - v^2/c^2}}$$

2.

23* Решение. Если электрон прошел через щель, то в плоскости самой щели координата x будет фиксирована с точностью $\Delta x \sim d$, где d - ширина щели. Однако в результате дифракции на щели волновая функция электрона ψ будет иметь максимумы и минимумы. Элек трон может быть обнаружен в любом месте, где $\psi \neq 0$. Наиболее интенсивным получится максимум нулевого порядка. Его угловая ширина равна 2θ, причем $d\sin\theta = \lambda$. Практически достаточно принять во внимание именно такой максимум. В этом приближении после прохождения через щель неопределенность Δp_x импульса электрона получится порядка $\Delta p_x = p\sin\theta = (h/\lambda)\sin\theta = h/d$. Таким образом, $\Delta x \Delta p_x \sim h$. Более определенное неравенство, которому должны удовлетворять Δx и Δp_x, с помощью этих соображений указать нельзя, поскольку не указан точный смысл самих величин Δx и Δp_x.

2.

24: При рассеянии фотона на электроне рассеянный фотон может попасть в любую точку плоскости изображения. Дифракционная картина в этой плоскости состоит из концентрических светлых и темных колец с центральным светлым кружком, называемым кружком Эйри, радиус которого равен $R \approx \lambda/\beta$ (рис. 142).

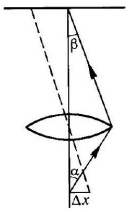


Рис. 142

Практически, рассеянный фотон может быть зафиксирован только внутри кружка, поскольку интенсивность там наибольшая. В этом приближении положение точки попадания фотона в плоскости изображения может быть определено с точностью порядка R. Неточность положения Δx электрона в предметной плоскости найдется из условия синусов Аббе $R\beta = \Delta x \sin\alpha$, т. е. $\lambda = \Delta x \sin\alpha$. При рассеянии фотона на электроне последний испытывает отдачу, в результате чего импульс электрона получает неконтролируемое приращение $\Delta p_x \sim \frac{h}{\lambda}\sin\alpha$. Таким образом, $\Delta x \Delta p_x \sim h$.

2.

25*. Решение. Пусть телом является идеально отражающее зеркало, а свет падает нормально на его поверхность. На основании законов сохранения энергии и импульса

$$\hbar\omega_0 + \frac{1}{2}Mv_0^2 = \hbar\omega + \frac{1}{2}Mv^2, \frac{\hbar\omega_0}{c} + Mv_0 = -\frac{\hbar\omega}{c} + Mv,$$

где M - масса тела, v_0 и v - его скорости до и после отражения света, ω_0 и ω - частоты падающего и отраженного фотонов. Переписав эти уравнения в виде

$$M\left(v^2 - v_0^2\right) = 2\hbar\left(\omega - \omega_0\right), M\left(v - v_0\right) = \frac{\hbar}{c}\left(\omega + \omega_0\right) \qquad (*)$$

почленным делением находим

$$v + v_0 = 2c\frac{\omega_0 - \omega}{\omega_0 + \omega}. \qquad ()$$

Для массивного зеркала $Mv^2/2 \gg \hbar\omega$. Поэтому $v \simeq v_0$, и тогда

$$v \simeq v_0 = c\frac{\omega_0 - \omega}{\omega_0 + \omega}.$$

Измерив частоты ω_0 и ω, можно по этой формуле вычислить скорость зеркала v. Частоту ω_0 можно считать измеренной точно. Тогда ошибка Δv в значении скорости будет определяться неточностью измерения частоты ω. Чтобы измерить ω с точностью $\Delta\omega$, надо производить измерение в течение времени Δt, удовлетворяющего условию $\Delta\omega\Delta t \sim 2\pi$. На основании $(^{**})$

$$\Delta v = -c\frac{2\omega_0\Delta\omega}{\left(\omega_0 + \omega\right)^2} \approx -c\frac{\Delta\omega}{2\omega_0}.$$

Так как моменты отражения фотона известны с ошибкой Δt, то неточность в значении скорости v поведет к ошибке Δx в определении координаты зеркала:

$$\Delta x \sim |\Delta v\Delta t| \sim \frac{c}{2\omega_0}|\Delta\omega\Delta t| \sim \frac{\pi c}{\omega_0}.$$

Согласно (*) при взаимодействии с фотоном зеркало получает неконтролируемое изменение импульса $\Delta p \sim 2\omega_0\hbar/$. Следовательно, $\Delta x\Delta p \sim 2\pi\hbar/c$ и

$$\Delta x\Delta p \sim 2\pi\hbar = h.$$

2.

26. $T > mv^2\sqrt{1 + (\Lambda/l)^2} - mc^2$, где $\Lambda = h/(mc)$ - комптоновская длина волны электрона (протона).

Для электрона $T > m_{\text{e}}c^2\Lambda_{\text{e}}/l_{\text{эл}} \approx 720$М или 7200 ГэВ во втором случае.

Для протона $T > m_{\text{p}}\text{c}^2\sqrt{1 + \left(\Lambda_{\text{p}}/l\right)^2} - m_{\text{p}}\text{c}^2 \approx 600$М или 8,2 ГэВ во втором случае.

2.

27. $d_{\min} = 2\sqrt{\frac{2Lh}{\sqrt{2m_{\text{p}}\varepsilon}}} \approx 8,5$mkM.

2.

28. $b = d + \frac{2hcl}{derB}$, откуда $b_{\min} = 2\sqrt{\frac{2hcl}{\text{er } B}} \approx 3,3 \cdot 10^{-4}$ cm.

2.

29. $d_{\min} = 2\sqrt{\frac{2h\tau}{m_e}} = 7,6$МКМ.

2.

30. $d \approx 2\sqrt{\frac{2hL}{\sqrt{3mkT}}} \approx 7,5$ мкм.

2.

31: $\Delta r \approx 2 \cdot 10^{-13}$ cm

Решение. Обмен «виртуальными» частицами - основной язык описания взаимодействия между реальными частицами в квантовой теории поля. Виртуальная частица - это частица, время жизни которой определяется соотношением неопределенностей, а не какими-либо другими физическими процессами. У виртуальной частицы есть энергия $\mathscr{E}$, импульс p, масса m. Однако для нее не выполняется обычное релятивисткое соотношение, и поэтому $\mathscr{E} \neq \sqrt{(pc)^2 + (mc^2)^2}$. Например, виртуальный фотон может обладать энергией и покоиться! Одна и та же частица, в зависимости от ситуации, может быть либо реальной, либо виртуальной. В связи с возникновением такой частицы в системе возникает неопределенность энергии $\Delta\mathcal{E}$, которая и определяет время жизни частицы $\boldsymbol{\tau} \sim \frac{\hbar}{\Delta}$. Через время $\tau \sim \frac{\hbar}{\Delta}$ поглащается либо самой испустившей ее реальной частицей или другой реальной частицей, и энергетический баланс в системе восстанавливается. В процессах испускания и поглощения выполняется закон сохранения импульса (хотя и направление импульса может и не совпадать с классическим).

При рассмотрении низкоэнергетических процессов, когда $^2 - p^2c^2 \ll \ll \left(mc^2\right)^2$, можно считать, что $\Delta\mathscr{E} \approx mc^2$, и тогда $\tau \sim \frac{\hbar}{mc^2}$. За это время частица может пройти расстояние $l \approx c\tau \sim \frac{\hbar}{mc} = \text{Å}_\text{K}$ - т. е. расстояние, равное комптоновской длине волны частицы. Это и есть радиус взаимодействия, обусловленный обменом виртуальными квантами.

2.

32. $\mathscr{E} \geq \hbar^2/8mr^2$. Для электрона в атоме $\mathscr{E} \geq 1 \ni$ В, для электрона в атомном ядре $\mathscr{E} \geq 10^{10}$ эВ $= 10^4$ МэВ. Электрон, будучи лептоном, может быть удержан в ядре только кулоновскими силами. Однако энергия взаимодействия $\sim Ze^2/R_{\text{яд}} \sim 1\text{М ВВ} \ll \mathscr{E} \sim 10^4$ МэВ.

2.

33: Решение. В полях такой напряженности из-за рождения виртуальных пар вакуум становится «поляризованной средой», а уравнения Максвелла теряют свойство линейности. Виртуальная пара живет время $\tau \sim \frac{\hbar}{\Delta\S} \sim \frac{\hbar}{2mc^2}$. Чтобы виртуальные частицы стали реальными, на длине $c\tau$ (на комптоновской длине волны) за счет работы электрического поля E дол-

жна набираться энергия, большая, чем $2mc^2$, т. е. $2mc^2 \approx eEc\tau \sim \frac{eE\hbar}{2mc}$, откуда $E \sim \frac{4m^2c^3}{e\hbar} \approx 2 \cdot 10^{14}$ ед. СГСЭ $= 6 \cdot 10^{16}$ В/с.

2.

34. $d = 0,61\frac{h}{A\sqrt{2meV}} = 0,024\text{НМ}$.

2.

35. $A = 0,83$ (в нерелятивистском приближении, $A = 1,73$). Числовая апертура A определяется из соотношения для минимально разрешаемого микроскопом расстояния $l \geqslant 0,61\frac{\lambda_e}{A}$, где $l = \frac{\hbar^2}{m_\mu e^2}$ - размер мезоатома, $\lambda_\text{e} = \frac{h}{p} = \frac{h}{\sqrt{(eV)^2 - (m_e c^2)^2}}$ - дебройлевская длина волны электрона.

2.

36. $A \approx \frac{h}{d\sqrt{2meV}} = 1,37 \cdot 10^{-2}$.

2.

37. $V = \frac{h^2}{2m_e e} \frac{1}{\lambda_{\text{опт}}^2} \left(\frac{\sin u_{\text{опт}}}{\sin u_{\text{эл}}} \right)^2 \approx 450$ В, где u - угловая апертура.

2.

38. $\bar{x} \approx \frac{4(\varepsilon+1)}{\varepsilon-1} r_1 \approx 76$Å, где $r_1 = \frac{\hbar^2}{me^2} = 0,53 \cdot 10^{-8}$ см - радиус первой боровской орбиты в атоме водорода. Энергия связи

$$\mathscr{E}_{\text{СВ}} \approx -\frac{me^4}{32\hbar^2} \left(\frac{\varepsilon-1}{\varepsilon+1} \right)^2 = \mathscr{E}_{\text{НОН}} \frac{1}{16} \left(\frac{\varepsilon-1}{\varepsilon+1} \right)^2 \approx -6,5 \cdot 10^{-4} \ni \text{ В}$$

где $\mathscr{E}_{\text{ион}} = \frac{me^4}{2\hbar^2} == 13,6$ эВ - энергия ионизации атома водорода.

2.

39: $\mathscr{E}_0 \approx 1,5 \left(\frac{k^2\hbar^2}{m} \right)^{1/3}, l \approx \sqrt[3]{\frac{\hbar^2}{km}}$.

Решение. В n-м стационарном состоянии квантовой системы, как следует из уравнений Шредингера, средние значения кинетической и потенциальной энергии удовлетворяют соотношению

$$\left\langle \widehat{T}_n \right\rangle + \left\langle \widehat{U}_n \right\rangle = \mathscr{E}_n$$

где $\widehat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}; \hat{U} = U(x); \mathscr{E}_n$ - полная энергия системы, а угловые скобки означают квантово-механическое среднее. Таким образом, $\frac{\langle \hat{p}^2 \rangle}{2m} + k\langle x \rangle = \mathscr{E}_n$. Для оценки энергии основного сос тояния воспользуемся тем, что в основном состоянии ($n = 0$) неопределенность координаты $\delta x \sim \langle x \rangle$, а неопределенность импульса $\delta p \sim \langle \hat{p} \rangle$ и $\langle \hat{p} \rangle^2 \sim \langle \hat{p}^2 \rangle$. Согласно соотношению неопределенностей получаем $\langle \hat{p} \rangle \langle x \rangle \sim \hbar$, откуда выражая, например $\langle x \rangle$ через $\langle p \rangle$, получим

$$\frac{\langle \hat{p} \rangle^2}{2m} + \frac{k\hbar}{\langle p \rangle} = {}_0$$

В основном состоянии энергия системы минимальна. Поэтому $\partial \mathscr{E}_0 / \partial \langle \hat{p} \rangle = 0$, т. е.

$$\frac{\langle \hat{p} \rangle}{m} - \frac{kh}{\langle \hat{p} \rangle^2} = 0$$

откуда $\langle \widehat{p} \rangle = p_0 = \sqrt[3]{km\hbar}$, а размер области локализации частицы в данной яме $l = \langle x \rangle = \frac{\hbar}{p_0} = \sqrt[3]{\frac{\hbar^2}{km}}$. Для энергии основного состояния получаем

$$\mathscr{E}_0 = \frac{3}{2m} (km\hbar)^{2/3} = 1,5 \left(\frac{k^2\hbar^2}{m} \right)^{1/3}$$

Приведем для сравнения точный результат, полученный из решения у равнения Шредингера для данного потенциала $\mathscr{E}_0 = 1,856 \left(\frac{k^2\hbar^2}{m} \right)^{1/3}$. Видно, что точность нашего приближенного подхода составляет примерно 20%.

2.

40*: Решение. Угол φ между направлением полета частиц и направлением излучения определяется из равенства

$$\cos\varphi = \frac{c}{nv}$$

Дифференцируем это выражение и заменяем дифференциалы конечными приращениями

$$\sin\varphi\Delta\varphi = \frac{c}{nv^2}\Delta v = \frac{c}{nm_e v^2}\Delta p$$

Электрон, находясь в слое вещества толщиной d, имеет неопределенность импульса $\Delta p \approx \hbar/d$, откуда следует неопределенность угла

$$\Delta\varphi \approx \frac{c\hbar}{dnm_e v^2 \sin\varphi}$$

2.

41: Решение. Чтобы имело смысл представление о классическом движении электрона по первой боровской орбите, необходимо выполнение соотношения $\Delta r \ll r_1$, где $r_1 = \hbar^2/me^2$ - радиус этой орбиты, а Δr - неопределенность положения электрона по радуису. Но тогда по соотношению неопределенностей соответствующая неопределенность в импульсе будет

$$\Delta p \approx \frac{\hbar}{\Delta r} \gg \frac{\hbar}{r_1} = \frac{me^2}{\hbar}$$

т. е. равна самому импульсу электрона $p = me^2/\hbar$. Однако по мере увеличения орбиты (увеличения квантового числа n), движение становится все более «классическим», что и постулируется принципом соответствия Бора.

2.

42. $\frac{l_n}{\lambda} = n, \lambda = \frac{h^2 n}{2\pi m e^2 Z} = 3,32 \cdot 10^{-8} \cdot \frac{n}{Z}$ cm.

2.

43: Решение. В стационарном состоянии квантово-механические средние значения кинетической и потенциальной энергий системы связаны соотношен ием

$$\langle T\rangle + \langle U\rangle = \mathscr{E}$$

где $\mathscr{E}$ - полная энергия системы.
B случае атома водорода $U = -\frac{e^2}{r}, T = \frac{p^2}{2\mu}$.

Если атом находится в основном состоянии, то $\Delta p \sim p; \Delta r \sim r$. Т.к. $\Delta p \Delta r \sim \hbar$, то $\mathscr{E} z \frac{\hbar}{2\mu r^2} - \frac{e^2}{r}$. Правая часть достигает минимума при

$$r = \frac{\hbar^2}{\mu e^2}$$

чем и определяется порядок величины размера атома водорода в основном состоянии. Соответствующая энергия

$$\mathscr{E} \geqq -\frac{\mu e^4}{2\hbar^2}$$

В случае двухатомной молекулья (если не учитывать ее вращения)

$$\langle T\rangle = \frac{\overline{p_x^2}}{2\mu}, \langle U\rangle = \frac{1}{2}\mu\omega_0^2\overline{x^2},$$

причем в силу соотношения неопределенностей в форме Вейля

$$\left(\overline{p_x^2} - \overline{p_x}^2\right)\left(\overline{x^2} - \bar{x}^2\right) \geqslant \frac{\hbar^2}{4}$$

В силу симметрии потенциальной ямы $\overline{p_x} = \bar{x} = 0$ и тогда
Таким образом,

$$\overline{p_x^2 x^2} \geqslant \frac{\hbar^2}{4}.$$

$$\frac{1}{2}\mu\omega_0^2\overline{x^2} + \frac{\hbar^2}{8\mu\overline{x^2}} \leqslant \mathscr{E}$$

Левая часть достигает минимума при $\overline{x^2} = \hbar/\left(2\mu\omega_0\right)$. Следовательно,

$$\mathcal{E} \geqslant \frac{1}{2}\hbar\omega_0.$$

Основное состояние - это состояние с минимально возможной энергией, и для него

$$\mathscr{E} = \frac{1}{2}\hbar\omega_0, \quad \overline{x^2} = \frac{\hbar}{2\mu\omega_0}.$$

Размер молекулы порядка $\sqrt{\frac{\hbar}{2\mu\omega_0}}$.

2.

44: $F \geqslant \sqrt{\frac{4\hbar m}{\tau^3}}$.

Решение. Минимальная сила, действие которой может быть определено по отклику свободной частицы (пробного тела) определяется квантово-механическими особенностями пробного тела и временем действия силы. При обнаружении малого внешнего воздействия на пробную квантово-механическую частицу требуется как минимум два измерения: начальной координаты и конечной (через время т). При этом мы не рассматриваем «снос» частицы $x = v_0\tau$ где v_0 - скорость свободной частицы, поскольку он не влияет на ответ.

Под действием силы частица движется с ускорением a, и за время т переместится на расстояние $l = \frac{a\tau^2}{2} = \frac{F_\tau^2}{2m}$. Этот результат справедлив и в квантовой механике. Зная координату частицы $x(0)$, т. е. в момент $t = 0$, мы могли бы знать положение частицы в момент $t = \boldsymbol{\tau} : x(\tau) = x(0) + l$. Следовательно, по крайней мере одно измерение координаты нам было бы необходимо.

Согласно основным представлениям квантовой механики при измерении вносится неконтролируемая неопределенность $\left\langle \Delta x_0^2 \right\rangle = \left\langle x^2 \right\rangle - \langle x \rangle^2$. В результате после измерения координаты возникает разброс в значении импульса $\left\langle \Delta p_x^2 \right\rangle$, который можно найти из соотношения неопределенностей в форме Вейля

$$\left\langle \Delta x_0^2 \right\rangle \left\langle \Delta p_x^2 \right\rangle \geqslant \frac{\hbar^2}{4}, \quad \text{откуда} \quad \left\langle \Delta p_x^2 \right\rangle \geqslant \frac{\hbar^2}{4\left\langle \Delta x_0^2 \right\rangle}$$

Через время т это приводит к неопределенности в пройденном расстоянии (конечную координату мы можем измерить сколь угодно точно).

$$\left\langle \Delta x_\tau^2 \right\rangle = \frac{\left\langle \Delta p_\lambda^2 \right\rangle \tau^2}{m^2} \geqslant \frac{\hbar^{22}_\tau}{4m^2\left\langle \Delta x_0^2 \right\rangle}.$$

Складывая обе дисперсии, в силу их статистической независимости получим

$$\left\langle \Delta x^2 \right\rangle = \left\langle \Delta x_0^2 \right\rangle + \left\langle \Delta x_\tau^2 \right\rangle \geqslant \left\langle \Delta x_0^2 \right\rangle + \frac{\hbar^{22}}{4m^2\left\langle \Delta x_0^2 \right\rangle}$$

Минимизируя полученное выражение по $\left\langle \Delta x_0^2 \right\rangle$, определяем неопределенность первого измерения координаты, которая обеспечит минимальную неопределенность пройденного за время т пути $\left\langle \Delta x_0^2 \right\rangle_{\min} = \hbar\tau/2m$. Это соответствует $\left\langle \Delta x^2 \right\rangle_{\min} = \hbar\tau/m$.

Силу можно будет зарегистрировать, если смещение l под действием силы окажется больше неопределенности пути

$$\frac{F\tau^2}{2m} \geqslant \sqrt{\frac{\hbar\tau}{m}}$$

откуда

$$F_{\min} = \frac{2m}{\tau^2}\sqrt{\frac{\hbar\tau}{m}} = \sqrt{\frac{4m\hbar}{\tau^3}}$$

2.

45: $F_{\min} = \sqrt{\frac{8\hbar^2 m}{\mathscr{E}_0 \tau^4}}$.

Решение. В этом случае мы измеряем энергию частицы до действия си лы и после. Первое измерение дает значение начальной энергии. Точность $\Delta\mathscr{E}$ такого измерения зависит от длительности измерения τ_1, т. е. $\Delta\mathscr{E} = \hbar/\tau_1$ (в принципе при достаточно большом τ_1 она может быть сделана сколь угодно малой). Поскольку полное время наблюдения ограничено величиной τ, то часть этого времени должна быть затрачена на измерение начальной энергии, а в оставшуюся часть времени $\tau - \tau_1$ будет происходить изменение энергии за счет работы силы F.

За время $\tau - \tau_1$ при условии $F\tau_1 \ll p_0$ изменение энергии

$$\Delta\mathscr{E}_0 = \frac{p_0 \Delta p}{m} = p_0 \frac{F(\tau - \tau_1)}{m}$$

Это изменение энергии можно обнаружить, если $\Delta\mathscr{E}_0 > \Delta\mathscr{E} = \hbar/\tau_1$, откуда

$$F \geqslant \frac{\hbar m}{p_0 \tau_1 (\tau - \tau_1)}.$$

Вводя $\mathscr{E}_0 = \frac{p_0^2}{2m}$ и минимизируя по τ_1, получаем

$$\tau_1 = \frac{\tau}{2} \quad \text{и} \quad F_{\min} = \frac{\hbar}{\tau^2}\sqrt{\frac{8m}{\varrho_0}}.$$

Заметим, что при подобных измерениях необходимо уменьшить все флуктуации энергии неквантовой природы (например, тепловые) до уровня меньше квантовых.

2.

46: Пороговая энергия рождения пары $\varrho = 2m_e c^2$. Эта энергия «появля-

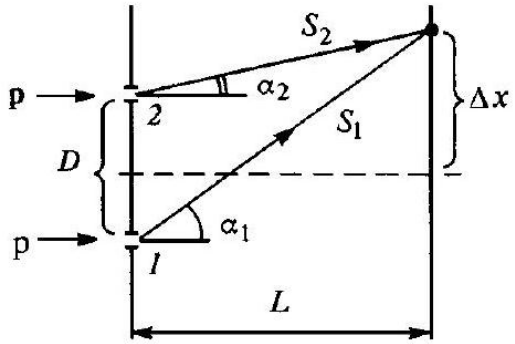


Рис. 143

ется» при попытке локализовать электрон в размере $\text{Å}_e/2$, где Å_e - комптоновская длина волны электрона. Действительно, при $\Delta x \simeq \frac{\Lambda_e}{2} = \frac{\hbar}{2m_e c}$ возникает неопределенность в энергии $\Delta\mathscr{E} = \frac{\hbar^2}{2m_e(\Delta x)^2}$, которая равна $2m_e c^2$. Таким образом в области $\sim \Lambda_e/2$ электрон не может рассматриваться как «точечный» объект.

2.

47. $t_{\text{изм}} \approx \frac{\hbar}{\mathscr{E}_\gamma} = 4 \cdot 10^{-20}\text{с}; \Delta\varrho \approx \frac{\hbar}{t_{\text{изм}}} = 15$ кэВ.

2.

48. Решение. Условие возникновения первого максимума $S_1 - S_2 = \lambda_{\text{дб}}$. Из геометрии разность хода (рис. 143)

$$S_1 - S_2 = \sqrt{\left(\frac{D}{2} + \Delta x\right)^2 + L^2} - \sqrt{\left(\Delta x - \frac{D}{2}\right)^2 + L^2} \approx \frac{D\Delta x}{L}$$

где использовано обычное условие эксперимента $L \gg D, \Delta x$.
Если электрон прошел через щель I, то изменение импульса экрана

$$|\Delta p_{x1}| = p\frac{\Delta x + D/2}{\sqrt{(\Delta x + D/2)^2 + L^2}}$$

а если через щель 2 , то

$$|\Delta p_{x2}| = p\frac{\Delta x - D/2}{\sqrt{(\Delta x - D/2)^2 + L^2}}$$

Чтобы определить по измерению импульса, через которую щель прошел электрон, нужно суметь различить по величине $|\Delta p_{x1}|$ и $|\Delta p_{x2}|$, т. е. точность измерений импульса должна быть лучше, чем

$$\Delta p_x = |\Delta p_{x1}| - |\Delta p_{x2}| \approx p\frac{\Delta x + D/2}{L} - p\frac{\Delta x - D/2}{2} = p\frac{D}{L}$$

Согласно соотношению неопределенностей

$$\delta x \delta p_x \sim h, \quad \text{откуда} \quad \delta x \sim \frac{h}{\delta p_x} \geqslant \frac{h}{\Delta p_x} = \frac{hL}{pD} = \frac{\lambda_{\text{ББ}}\, L}{D}.$$

Так как $\lambda_{\text{дБ}} = \frac{D\Delta x}{L}$, то $\delta x \geqslant \Delta x$. Тем самым неопределенность в положении щелей (обе щели смещаются как целое вместе с экраном) будет больше, чсм масштаб интерференционного расщепления, и картина размоется.

2.

49*: Решение. Пока расстояние d между расщепленными пучками меньше $0,61\lambda_{\text{ф}}$ (результат, хорошо известный в оптике как предельное разрешение двух светящихся точек), определить, каким путем движется атом, невозможно. Поэтому первое размытие картины произойдет при $d = 0,61\lambda_{\text{ф}}$. Так как угол дифракции мал, то, как следует из рис. 144 , размытие интерференционной картины произойдет при расстоянии между пучками

$$d \approx z\theta = z\frac{\lambda_{a\ \text{В}}}{a} = \frac{z}{a}\frac{h}{p}.$$

Поэтому

$$z = 0,61\lambda_{\Phi}\frac{a}{\lambda_{\text{дБ}}} = \frac{0,61\lambda_{\phi} aMv}{h} = 6 \text{ mm}.$$

Следует отметить, что при таком способе измерения координат атомов изза их большой массы $\Delta p_{\perp}$, возникающее из соотношения неопределенностей, очень мало.

2.

50. $F = \frac{n_0 h}{4d^2}\left(\lambda_2^2 - \lambda_1^2\right) \approx 5 \cdot 10^{-21}$ дин, где $\lambda_2 = 4\text{Å}$ и $\lambda_1 = 2\text{Å}$ (упруго рассеиваться будут все нейтроны с длиной волны $\lambda \leqslant 4\text{Å}$).

2.

51. $v = \frac{h}{M\lambda} = 2,77 \cdot 10^4$ cm/c, где $\lambda = \frac{d\Delta}{l}$ - длина волны фуллеренов.

2.

52. Скорость тримеров и димеров одинакова: $v = \frac{h}{\theta MNd} = 1,8 \cdot 10^6$ cm/c, где N - число ато-

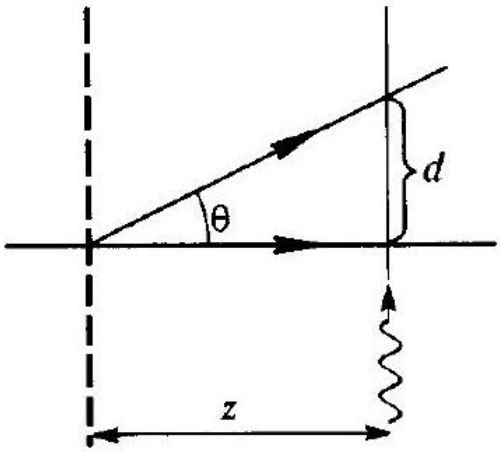


Рис. 144 мов гелия в кластере.

2.

53. $\Delta\varphi \simeq \sqrt[4]{\frac{\hbar^2}{m^2 l^3 g}}; \Delta L \simeq \left(\hbar^2 m^2 g l^3\right)^{1/4}$. Легко проверить, что $\Delta\varphi\Delta L \simeq \hbar$.

2.

54*: Решение. Флуктуация энергии в системе осцилляторов $\Delta\mathscr{E} = \Delta N\hbar\omega$; в свою очередь, $\Delta t = \frac{\Delta\varphi}{\omega}$. Поэтому $\frac{\Delta\mathscr{E}\Delta t}{\hbar} = \Delta N\Delta\varphi = 1$.

18.1.18 Basic problems about atoms in fields 1

(первые отсюда задачи в оптику скорее всего перенесу)

О3.1-6.1 Вращение диска светом

Пучок циркулярно поляризованного света с длиной волны $\lambda = 0,5$ мкм падает на зачерненный диск, подвешенный на тонкой нити так, что он может совершать крутильные колебания относительно оси. Измеряется установившийся угол поворота. Диск имеет массу $m = 1$ г и радиус $r = 5$см. Найти период собственных колебаний диска T, если при мощности светового потока $N = 10$ Вт угол поворота диска составил $\alpha = 1''$.

6.

1. $T = 2\pi r\sqrt{\frac{\pi amc}{N\lambda}} = 5$ мин.

(??? непонятно, почему в разделе про магнетизм задача. По идее через давление света все решается. нужно переучивать)

О3.1-6.2 Вращение пластины светом

Абсолютно черная пластинка площадью $S = 10$ см ^{2} освещается монохроматическим светом с длиной волны $\lambda = 600$, поляризованным по кругу. Интенсивность света равна $\vartheta = 30\text{Br/cm}^2$. Какой вращающий момент M испытывает пластинка? Зависит ли M от распределения интенсивности в пучке? Как изменится вращающий момент, если черную пластинку заменить на кристаллическую пластинку в $\lambda/4$? Какую надо взять кристаллическую пластинку, чтобы вращающий момент M удвоился?

6.

2. $M = \frac{\mathscr{I} S \lambda}{2\pi c} = 0,95 \cdot 10^{-6}$ дин $\cdot$ см. От распределения интенсивности в пучке M не зависит. Для пластинки в $\lambda/4$ вращающий момент такой же, как и для поглощающей пластинки. Вращающий момент удвоится, если взять пластинку в $\lambda/2$.

О3.1-6.3 Вращательный момент

Эллиптически поляризованный параллельный световой поток с длиной волны $\lambda = 600$ нм и интенсивностью $\mathscr{I} = 30\text{В}/\text{см}^2$ падает перпендикулярно на абсолютно черную пластинку. Площадь поперечного сечения светового потока $S = 10\text{см}^2$. Отношение длин главных полуосей эллипса поляризации в световом пучке составляет $a/b = 2$. Найти вращающий момент M, который испытывает пластинка при поглощении света.

6.

3. $M = \frac{gS\lambda}{2\pi c} \frac{2ab}{a+b} = 0,76 \cdot 10^{-6}$ дин $\cdot$.

О3.1-6.4 Двоякопреломляющая пластинка

Поляризованный по правому кругу световой поток с длиной волны $\lambda = 500$ нм, интенсивность которого составляет $\mathscr{I} = 1,4 \cdot 10^6 \text{pr}/\left(\text{с} \cdot \text{см}^2\right)$ (такой интенсивностью обладает солнечное излучение на границе земной атмосферы), падает на двоякопреломляющую пластинку в $\lambda/2$. Как будет поляризован свет после прохождения пластинки? Определить вращающий момент на единицу площади (M/S) такой пластинки.

6.

4. Свет будет поляризован по левому кругу.

$$\frac{M}{S} = \frac{g\lambda}{\pi c} = 7,7 \cdot 10^{-9} \text{ дин } /$$

О3.1-6.5 Вращательный момент

На кварцевую пластинку в $\lambda/4$ перпендикулярно падает пучок линейно поляризованного света с длиной волны $\lambda = 628$ нм и мощностью $N = 3\text{В}$. При каких условиях пластинка будет испытывать вращающий момент и каковы его значение и направление?

6.

5. Максимальный вращающий момент возникает, когда главные направления пластинки ориентированны под углом 45° к плоскости поляризации света.

$$M = \frac{N\lambda}{2\pi c} = 10^{-8} \text{ дин } \cdot .$$

О3.1-6.6 Вращающийся момент по максимумам и минимумам

Некогерентная смесь естественного и линейно поляризованного света с длиной волны $\lambda = 500$ нм и интенсивностью $\mathscr{J} = 1,4 \cdot 10^6$ эрг/ $\left(\text{с}^2\text{см}^2\right)$ (такой интенсивностью обладает солнечное излучение на границе земной атмосферы) падает на двоякопреломляющую пластинку в $\lambda/4$. Определить вращающий момент на единицу площади (M/S) такой пластинки, если направление колебаний в линейно поляризованном свете составляет угол 45° с главными направлениями пластинки. Известно, что при анализе падающего из тучения с помощью поляризатора соотношение $\tau_{\max}/\mathscr{E}_{\min} = 3$.

6.

6. Из условий $_{\max}/\mathscr{C}_{\min} = 3$ следует, что линейно поляризованный свет переносит половину всей мощности.

$$\frac{M}{S} = \frac{g\lambda}{4\pi c} = 1,9 \cdot 10^{-9} \text{ дин } /.$$

О3.1-6.7 Вращение решетки

Параллельный пучок монохроматического излучения (длина волны в вакууме $\lambda = 496$ мкм), поляризованного по кругу, падает нормально на решетку, изготовленную в виде натянутых проволочек с расстоянием между ними $d \ll \lambda$. При таких условиях решетка полностью пропускает излучение, поляризованное так, что электрический вектор направлен перпендикулярно проволочкам, и отражает излучение с поляризацией, повернутой на 90°. Найти вращающий момент M и силу F, действующих на решетку, если интенсивность потока в пучке $\vartheta = 10\text{В/см}^2$, а облучаемая поверхность решетки $S = 10\text{см}^2$.

6.

7* $M = \frac{\mathscr{J} S\lambda}{2\pi c} \approx 3 \cdot 10^{-4}$ дин ·; $F = \frac{\mathscr{J} S}{c} \approx 0,03$ дин.

Решение. Момент импульса проходящей и отраженной волн равен нулю в силу линейной поляризации. Согласно закону сохранения момента импульса $\Delta L_{\text{реш}} = -\Delta L_{\text{фот}}$ (изменению момента импульса фотонов).

Вращающий момент $M = \frac{\Delta L_{\text{dx}}}{\Delta t} = \frac{\hbar \mathscr{J} S \Delta t}{\hbar\omega \Delta t} = \frac{\mathscr{J}\mathscr{S}}{\omega} = \frac{\mathscr{S}\mathscr{S}}{2\pi c} \approx 3 \cdot 10^{-4}$ дин ·с.
Сила давления F обусловлена изменением импульса той части потока, которая испытывает отражение. Поэтому

$$F = 2\frac{\hbar\omega}{c}\frac{\mathscr{A} S}{2\hbar\omega} = \frac{S}{c} \approx 0,03 \text{ дин.}$$

О3.1-6.8 Вращение цилиндра Фарадея

Пучок продольно поляризованных по спину электронов с током 100 А и кинетической энергией 100 кэВ поглощается цилиндром Фарадея. Определить силу и крутящий момент, действующие на цилиндр. Пучок электронов направлен параллельно оси цилиндра.

6.

8. $F = p\frac{g}{e} = 1,12 \cdot 10^4$ дин, где $p = \frac{1}{c}\sqrt{T\left(T + 2mc^2\right)} = 1,78 \cdot 10^{-17}\Gamma \cdot \text{с}/; M = \frac{\hbar}{2e} = 3,3 \cdot 10^{-7}$ дин · см.

О3.1-6.9 Вращение цилиндра

С какой угловой скоростью ω и в каком направлении должен начать вращаться цилиндр, подвешенный в магнитном поле B, направленном параллельно его оси вертикально вверх, если изменить направление поля на обратное? Считать, что цилиндр намагничивается до насыщения. (Момент импульса электрона в атоме равен l, число атомов в цилиндре N, момент инерции цилиндра I.)

6.

9. $\omega = \frac{2Nl}{I}$, цилиндр закрутится против часовой стрелки (вектор ω направлен вверх).

О3.1-6.10 Вращение цилиндра

Какое значение для ω следует ожидать в упрощенном опыте Эйнштейна-де Гааза (предыдущая задача), если длина цилиндра $L = 1$см, его масса $m = 1$, цилиндр сделан из железа и если предположить, что момент импульса каждого атома равен таковому для электрона на первой боровской орбите?

6.

10. $\omega = \frac{2N_A h}{Am} Lp = 1,1 \cdot 10^{-3}\text{с}^{-1}$, где N_A - число Авогадро, A - атомная масса железа [г/моль], ρ - его плотность.

О3.1-6.11 Опыт Штерна-Герлаха с водородом

На сколько компонент расщепится при проведении опыта Штерна-Герлаха пучок атомов водорода?

6.

11. На два ($2S + 1 = 2$).

О3.1-6.12 Опыт Штерна-Герлаха с натрием

Пучок атомов натрия, находящихся в основном состоянии, вылетает из печи, температура которой $T = 350$ К. Пучок расщепляется в поперечном неоднородном магнитном поле с градиентом $dB/dx = 50$ Тл/м на пути $l = 1$ см. Детектор удален от магнита на расстояние $L = 6,5$ м. Найти расстояние s между пятнами на экране.

6.

12* $s = 2\mu_\text{б} \frac{dB}{dx} \frac{l(L+l/2)}{3kT} \approx 0,4$ см.
Решение. В области магнита на атом действует постоянная сила

$$F_x = \mu_B \frac{dB}{dx}$$

где μ_B - проекция магнитного момента атома на направление поля B

$$\mu_B = m_J g \mu_\text{Б}$$

где $g = \frac{3}{2} + \frac{S(S+1)-L(L+1)}{2J(J+1)}$ - фактор Ланде. В основном состоянии атома Na $L = 0, S = 1/2, J = 1/2, g = 2$, и $F_x = \pm\mu_\text{б} \frac{dB}{dx}$. За время $t = \frac{l}{v}$ смещение частицы $x_1 = \frac{at^2}{2} = \frac{F_x}{2m} \frac{l^2}{v^2}$, а скорость на выходе $v_x = \frac{F_x}{m} \frac{l}{v}$ ($v_x \ll v$, в чем убедимся ниже). Вне магнита атом движется по инерции и $x_2 = x_1 + v_x \frac{L}{v} = \frac{F_x}{mv^2} l \left(\frac{l}{2} + L\right)$.
За время $t = l/v$ атомы приобретают скорость

$$v_x = \pm\mu \frac{dB}{dx} \frac{l}{mv} \approx \pm 20\text{с/с}$$

приводящую к смещению пучков на детекторе

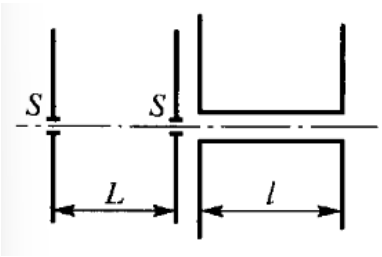
$$x_2 = \pm\mu_\text{Б} \frac{dB}{dx} \frac{l(l/2 + L)}{mv^2}$$

Средняя кинетическая энергия атомов в пучке равна $\overline{\frac{mv^2}{2}} = \frac{3}{2}kT$, откуда $v \simeq 600$ м/с $\gg v_x$, а искомое расстояние между пятнами на детекторе

$$s = 2x_2 = 2\mu_\text{Б} \frac{dB}{dx} \frac{l(l/2 + L)}{3kT} \approx 4 \text{ mm}$$

О3.1-6.13 Магнит Штерна-Герлаха и диафрагмы

Пучок атомов лития в основном состоянии с максимальной кинетической энергией $T = 0,1$ эВ проходит через магнит типа Штерна-Герлаха длиной $l = 6$см с градиентом поля $dB/dx = 5 \cdot 10^4$Гс/cm. Сразу за магнитом расположена система из двух одинаковых диафрагм S диаметром d, находящихся на расстоянии $L = 1$ м одна от другой



При какой минимальной величине диаметра $d_{\min}$ компоненты разделенного пучка пройдут через систему диафрагм?

Solution

(???)

О3.1-6.14

Пучок атомов ванадия ($A = 50$), находящихся в состоянии ${}^4F_{3/2}$, пропускается через сильное неоднородное магнитное поле. На сколько компонент разобьется такой пучок?

На какой угол разойдутся соседние компоненты пучка, если участок с неоднородным полем имеет протяженность $l = 25$см, градиент поля в нем $dB/dx = 5 \cdot 10^4$Гс/cm, а скорость атомов $v = 500$ м/с?

Solution

(???)

О3.1-6.15 Коллиматор и магнит

Параллельный пучок нейтронов с энергией $T = 0,025$ эВ проходит через коллимирующую щель шириной $d = 0,1$ мм и затем через зазор в магните Штерна-Герлаха длиной $L = 1$ м. Оценить значение градиента поля dB/dx, при котором угол магнитного отклонения компонент пучка равен углу дифракционного уширения. Магнитный момент нейтрона $\mu_{\text{n}} = 9,66 \cdot 10^{-24}$ эрг/Гс.

Solution

(???)

О3.1-6.16 Расщепление пучка нейтронов

В опытах Шалла (1968 г.) наблюдалось расщепление пучка нейтронов на два пучка при преломлении на границе однородного магнитного поля. Найти малый угол θ между направлениями преломления пучков. Однородное магнитное поле имеет индукцию $B = 2,5$ Тл. Нейтроны с дебройлевской длиной волны $\lambda = 0,5$ нм падают под углом $\varphi = 30^\circ$ к достаточно резкой границе магнитного поля.

Solution

(???)

О3.1-6.17 Мультиплетность

Определить возможную мультиплетность атомов H, He, Li, Mg, Fe, Hg, U, Cl.

Solution

(???)

О3.1-6.18 Мультиплетность

Какова возможная мультиплетность Sr^+, Li^+, Ca^+, c^{++}, O^{4+}?

Solution

(???)

О3.1-6.1 Мультиплетность

Какова наивысшая мультиплетность атомов элементов третьей группы?

Solution

(???)

О3.1-6.20 Дублет натрия (!!!!!)

Желтый дублет Na возникает при переходе электронов $3^2P \to 3^2S$ и соответствует длинам волн $\lambda_1 = 5896$Å и $\lambda_2 = 5890$Å. Найти энергетическое расстояние $\Delta\S$ между соответствующими подуровнями терма 3^2P (мультиплетное расщепление). Оценить среднюю величину магнитного поля B, действующего на «оптический» электрон.

Solution

(???)

О3.1-6.21 Переход $P \to S$

При переходе $P \to S$ из возбужденного состояния атома в основное испускается дублет $\lambda_1 = 455,1$ нм и $\lambda_2 = 458,9$ нм. Какие линии, соответствующие переходу ${}^2S_{1/2} \to {}^2P_{3/2}$, будут наблюдаться в спектре поглощения газа, состоящего из таких атомов, при наложении магнитного поля 50κ при температуре $T = 0,5$ К?

Solution

(?? про Зеемана тут???? пока не очень вижу)

Решение Первое, с чем определимся это то какой это эффект Зеемана - в сильном или слабом поле? Считаем характерные энергии спин-орбитального взаимодействия и взаимодействия с магнитным полем:

$$U_{LS} = \frac{hc}{\lambda^2}\Delta\lambda = 2 \cdot 10^{-2\text{В}}\text{В}$$
$$U_B = \mu B = 3 \cdot 10^{-4\ni}\text{В}$$
$$kT = 4 \cdot 10^{-5\text{В}}$$

То есть это слабое поле, при этом все атомы сидят в нижнем положении по энергии, а сама задача стоит о поглощении а не испускании. А дальше смотрим на известную нам из теории структуру линий для этого эффекта из теории и просто записываем разницы энергий:

$$E_B = \mu B\left(g_1 m_{j1} - g_2 1 m_{j2}\right)$$
$$E_B = \mu B \begin{cases} 4/3 \cdot 1/2 - 2 \cdot (-1/2) = 5/3 \\ 4/3 \cdot (-1/2) - 2 \cdot (-1/2) = 1/3 \\ 4/3 \cdot (-3/2) - 2 \cdot (-1/2) = -1 \end{cases}$$

(!!!! с температурой еще разберусь, в 1ю часть занесу!!!!)

О3.1-6.22

В отсутствии магнитного поля газ поглощает электромагнитное излучение с длиной волны $\lambda = 500$ нм, соответствующее переходу из основного состояния $^2P_{1/2}$ в возбужденное $^2D_{3/2}$. Как изменится спектр поглощения этого газа в окрестности этой длины волны при наложении магнитного поля $B = 2$ кГс при температуре, близкой к комнатной? В спектре испускания этого газа в окрестности $\lambda = 500$ нм наблюдается дублет с $\Delta\lambda = 0,5$, соответствующий переходам $^2D_{3/2} \to {}^2P_{1/2}, {}^2D_{3/2} \to {}^2P_{3/2}$.

18.1.19 Basic problems about atoms in fields 2

О3.1-6.23 Расщепление

На сколько компонент расщепится в слабом магнитном поле мультиплет с заданным полным моментом J?

О3.1-6.24 Расщепление

Найти энергетическое расщепление термов атомов группы щелочных металлов, помещенных в слабое магнитное поле.

О3.1-6.25 Расщепление

На сколько компонент расщепится в слабом магнитном поле линия Na, отвечающая переходу $^2F_{7/2} \to {}^2D_{5/2}$?

О3.1-6.26 Расщепление

Найти число компонент сложного эффекта Зеемана линии Na, указанной в предыдущей задаче, которые поляризованы по магнитному полю.

О3.1-6.27 Расщепление

Определить расщепление спектральной линии $^2P_{3/2} \to \to {}^2S_{1/2}$ в слабом магнитном поле. Для натрия эта линия является коротковолновой компонентой ($\lambda = 589,0$ нм) двойной линии D с $\Delta\lambda = 0,6$ нм. Какие магнитные поля в этом случае являются слабыми?

О3.1-6.28 Расщепление

На сколько уровней расщепится в сильном магнитном поле терм с $L = 3$ и $S = 0$? Какова разность энергий соседних уровней?

О3.1-6.29 Расщепление

На сколько компонент расщепится в магнитном поле спектральная линия, связанная с оптическим переходом $L = 3 \to L = 2$ (излучается $E1$-фотон), при простом эффекте Зеемана?

О3.1-6.30 Направления поля

В сильном магнитном поле B при наблюдении в направлении, перпендикулярном полю (поперечный эффект Зеемана), в спектре излучения имеется три линейно поляризованных линии: несмещенная спектральная линия с длиной волны λ и электрическим вектором, направленным вдоль магнитного поля, и две смещенные - с Электрическим вектором $\mathbf{E} \perp \mathbf{B}$. Это излучение пропускается через два скрещенных поляризатора, между которыми находится анизотропная кристаллическая пластинка с заданными Δn и d. Оптическая ось пластины составляет углы 45° с направлениями поляроидов. При какой величине магнитного поля в спектре излучения будут видны лишь две крайние линии?

О3.1-6.31 Дополнительная энергия от поля

Атомарный водород помещен в магнитное поле 2 Тл, много большее характерного поля атома, т. е. магнитного поля атома, действующего на электрон. Определить максимальную дополнительную энергию (в эВ), которую приобретает атом в состоянии с $n = 3$ и нарисовать картину расщепления этого уровня.

О3.1-6.32 Разрешение простого эф. Зеемана

Наблюдается простой поперечный эффект Зеемана в магнитном поле $B = 5000$ Гс. Какова должна быть минимальная длина L дифракционной решетки, чтобы разрешить все линии зеемановского триплета?

О3.1-6.33

При какой минимальной ширине L дифракционной решетки, имеющей $n = 600$ линий/мм, можно разрешить в первом порядке дублет простого эффекта Зеемана для спектральной линии $\lambda = 0,612$ мкм? Напряженность магнитного поля $B = 10$ кГс.

О3.1-6.34

С помощью эшелона Майкельсона наблюдается зеемановское расщепление D-линии натрия в магнитном поле $B = 5000$Гс (сложный эффект). Какова должна быть максимальная толщина 51 d пластины, чтобы эшелон был пригоден для исследования расщепления? Показатель преломления материала пластины $n = 1,5$. Под D-линиями Na понимают две линии нерасщепленного полем дублета $3^2P_{3/2} \to 3^2S_{1/2}$ и $3^2P_{1/2} \to 3^2S_{1/2}$

О3.1-6.35

Определить верхний предел расстояния $L_{\max}$ между зеркалами интерферометра Фабри-Перо, чтобы с его помощью можно было исследовать (без перекрытия спектров разных порядков) простой эффект Зеемана в магнитном поле $B = 1$ Тл.

6.

35. $L_{\max} = \frac{2\pi m_e c^2}{eB} \approx 1,1$ cm.

О3.1-6.36

Какой эффект Зеемана - простой или сложный - наблюдается при расщеплении спектральной линии ${}^1D_2 \to {}^1F_3$ в магнитном поле $B = 10^4$ Гс? В каких пределах должно лежать расстояние L между зеркалами интерферометра Фабри-Перо, чтобы обнаружить и исследовать зеемановское расщепление рассматриваемой линии? Зеркала посеребрены так, что эффективное число отражений между ними $N_{\text{eff}} = 20$.

6.

36. Нормальный (простой), так как рассматриваемая линия - синглет. Разрешающая способность интерферометра $N_{\text{эфф}}$ m должна быть не меньше $\frac{\omega}{\delta\omega}$, где $\delta\omega = \Omega = \frac{eB}{2m_e c}$. Величина $\delta\lambda = \frac{2\pi c}{\omega^2}\delta\omega$ должна быть меньше дисперсионной области λ/m, где $m = L/\lambda$ - порядок спектра. Из этих условий получаем

$$\frac{2\pi m_e c^2}{eBN_{\text{эфф}}} < L < \frac{2\pi m_e c^2}{eB}$$

или в рассматриваемом случае 0,54 мм $< L < 10,7$ мм.

О3.1-6.37

Найти зеемановское расщепление $\Delta\omega$ спектральной линии

6.

37: $\Delta\omega = \frac{eB}{2m_e c}\left(\pm\frac{13}{15}; \pm\frac{11}{15}; \pm\frac{1}{15}\right)$; (6 компонент).

Решение. Определим g-факторы состояний ${}^2D_{3/2}$ и ${}^2P_{1/2}$. Квантовые числа состояния ${}^2D_{3/2}$ соответственно равны $J_1 = 3/2; L_1 = 2; S_1 = 1/2$. Квантовые числа состояния ${}^2P_{1/2}$ соответственно равны $J_2 = 1/2, L_2 = 1, S_2 = 1/2$.

$$g_1 = \frac{3}{2} + \frac{S_1(S_1+1) - L_1(L_1+1)}{2J_1(J_1+1)} = \frac{4}{5}$$

Аналогично, $g_2 = 2/3$. Таким образом, состояние $^2D_{3/2}$ расщепляется в магнитном поле на 4 подуровня (рис. 166) по m_J. Состояние $^2P_{1/2}$ расщепляется по m_J на два подуровня. Поскольку $g_1 \neq g_2$, то спектральная линия расщепляется в магнитном поле B в соответствии с правилами отбора ($\Delta m_J = 0, \pm 1$) на шесть компонент. Это сложный эффект Зеемана. Общая формула для расчета расщепления

$$\omega = \omega_0 + \frac{\mu_{\mathrm{E}} B}{\hbar}\left(g_1 m_{J1} - g_2 m_{J2}\right)$$

или

$$\Delta\omega = \omega - \omega_0 = \frac{eB}{2m_{\mathrm{e}}c}\left(g_1 m_{J1} - g_2 m_{J2}\right) = \Omega\left(\pm\frac{13}{15}; \pm\frac{11}{15}; \pm\frac{1}{15}\right)$$

где Ω - ларморовская частота.

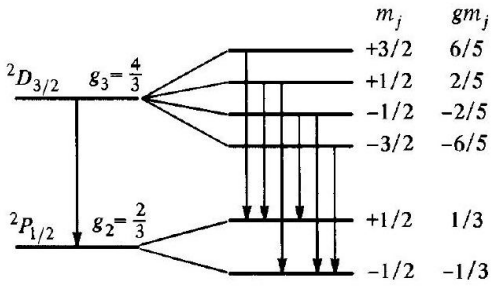


Рис. 166

О3.1-6.38

Цезий принадлежит к числу щелочных металлов. При $P \to S$ - переходе в атомарном цезии испускается дублет, состоящий из двух линий: $\lambda_{\mathrm{I}} = 0,4555$ мкм и $\lambda_2 = 0,4593$ мкм. Найти расщепление термов этого дублета в магнитном поле. Какими формулами описывается в этом случае расщепление линий в магнитном поле с индукцией $B = 3$ Тл: формулами для нормального или аномального эффектов Зеемана?

6.

38. Зеемановское расщепление в магнитном поле $\Delta\lambda_B = \frac{\Delta\S\lambda^2}{2\pi\hbar c} \sim \sim \frac{\mu_5 B\lambda^2}{2\pi\hbar c} \sim 0,1\text{Å} \ll \Delta\lambda = 38\text{Å}$ (расщепление в результате спин-орбитального

взаимодействия). Поэтому поле слабое, эффект аномальный (сложный). Од на линия дублета расщепится на шесть линий, другая - на четыре (см. задачу 6.34).

О3.1-6.39

В спектре лития две первые линии главной серии принадлежат переходам $2^2P_{1/2} \to 2^2S_{1/2}$ и $2^2P_{3/2} \to 2^2S_{1/2}$. Длины волн этих линий равны $\lambda_1 = 0,670780$ мкм и $\lambda_2 = 0,670795$ мкм. Оценить индукцию B магнитного поля, которое создает орбитальное движение электрона в атоме лития в состоянии $2P$.

О3.1-6.40

Так как атом мюония $(\mu^+ e^-)$состоит из двух точечных» частиц, то для него не нужно вводить при расчете уровней энергии никаких поправок на конечный размер ядра. В результате очень точных измерений частоты перехода $1^2S_{1/2} \to 2^2S_{1/2}$, проведенных в 1992 году, было получено значение $v = 2455529$ Гц. Найти из этих данных отношение массы мюона к массе электрона.

О3.1-6.41

Оценить расщепление уровня $n = 2, l = 1$ водорода из-за магнитного взаимодействия спина с его орбитальным движением. Ук а з а и е. Энергия взаимодействия спина с орбитой пропорциональна cos $\hat{\mathrm{l}}\mathrm{s}$, где 1 - орбитальный и $\mathbf{s}$ - спиновый моменты.

18.1.20 Basic problems about atoms in fields 3

О3.1-6.42

Оценить дублетное расщепление первой линии серии Лаймана в спектре излучения водорода, предполагая, что состояние $n = 1$ не расщепляется, а состояние $n = 2$ расщеплено на величину, вычисленную в задаче 6.41.

(дальше не выгружал пока что, хватает над чем подумать.)

6. SOLUTIONS Спин. Атом в магнитном поле. Эффект Зеемана. Магнитный резонанс.

6.

13. $d_{\min} = \mu_{\text{К}} \frac{dB}{dx} \frac{lL}{T} \left(1 + \frac{l}{2L}\right) = 1,79$ см.

6.

14. Пучок разобьется на четыре компоненты. Угол между ними $\Delta\varphi = g\mu_\sigma \frac{dB}{dx} \frac{l}{Am_{\text{p}}v^2} \approx 2 \cdot 10^{-2}$ рад $\approx 1,2°$.

В области магнита на атом действует постоянная сила $F_x = \mu_B \frac{dB}{dx}$, где μ_B - проекция магнитного момента атома на направление поля $B\mu_B = m_J g \mu_{\text{Б}}$, где $g = \frac{3}{2} + \frac{S(S+1)-L(L+1)}{2J(J+1)}$ - фактор Ланде. Из определения спектроскопического символа ${}^{2S+1}F_J$ имеем $S = 3/2; J = 3/2$ и $L = 3$, поэтому g-фактор (фактор Ланде) $g = 2/5$.

6.

15. $\frac{dB}{dx} = \frac{4\pi\hbar}{\mu_{\text{n}} Ld} \sqrt{\frac{T}{2m_{\text{n}}}} \approx 150$Гс/cm.

6.

16* $\theta = \frac{1{,}91\mu_{\text{яд}} B\lambda^2}{2\pi^2\hbar^2} m_{\text{n}} \operatorname{tg}\varphi = 86$ мкрад $\approx 3'$.

Решение. Выберем координатные оси таким образом: поле $\mathbf{B}$ направлено по оси Z, а нормаль к области поля есть ось X (рис. 160). Потенциальная энергия нейтрона в магнитном поле

$$U = -\boldsymbol{\mu}\mathbf{B} = -\mu_{\text{яд}}\, B_z g_{\text{sn}} m_s$$

где $\mu_{\text{яд}}$ - ядерный магнетон Бора, $g_{sn} = -3,82$ - спиновый g-фактор нейтрона (аналог фактора Ланде для свободного электрона),$m_s = \pm\frac{1}{2}$.

Поскольку потенциальная энергия однородна и различна в областях $x < 0$ и $x > 0$, то это приводит к силам, действую- щим на нейтрон в направленнии по нормали к поверхности, а вдоль поверхности силы не действуют. Поэтому касательная компонента импульса нейтрона будет сохраняться ($m \equiv m_{\text{n}}$ масса нейтрона):

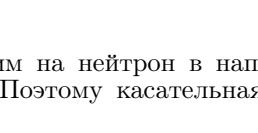


Рис. 160

$$mv_{\text{I}} \sin\varphi = mv_{\text{II}} \sin\psi, \quad \text{т. е.} \quad \frac{\sin\varphi}{\sin\psi} = \frac{v_{\text{II}}}{v_{\text{I}}} = n$$

Получили аналог оптического закона преломления. Из закона сохранения энергии

$$\frac{mv_{\text{I}}^2}{2} = \frac{mv_{\text{II}}^2}{2} \pm U_0 \quad \text{получаем} \quad n = \sqrt{1 \mp \frac{2U_0}{mv_{\text{I}}^2}}$$

Возможен другой способ получения выражения для показателя преломления нейтронов. На рис. 161 приведен график зависимости потенциальной энергии нейтрона $U(x)$ от координаты x. Из рисунка видно, что данную задачу можно рассматривать как задачу о надбарьерном отражении нейтронной волны де Бройля. Волновая функция нейтрона $\psi = Ae^{i\mathbf{kr}} = Ae^{ik_x x}$ ($k_y = \text{const}$ и $k_z = \text{const}$). Используя известный

результат задачи (3.25), за-

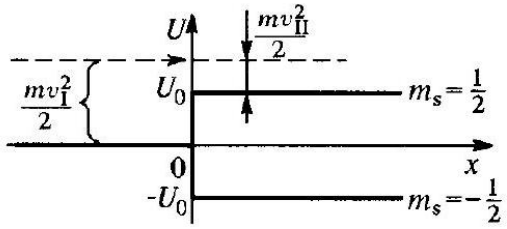


Рис. 161 пишем коэффициент отражения

$$R=\left(\frac{k_{xI}-k_{xII}}{k_{xI}+k_{xII}}\right)^2=\left(\frac{k_I\cos\varphi-k_{II}\cos\psi}{k_I\cos\varphi+k_{II}\cos\psi}\right)^2=\left[\frac{\cos\varphi-(k_{II}/k_I)\cos\psi}{\cos\psi+(k_{II}/k_I)\cos\psi}\right]^2$$

Если сравнить это выражение с соответствующей формулой Френеля, то получим, что

$$n=\frac{k_{II}}{k_I}=\sqrt{1\mp\frac{2mU_0}{\hbar^2k_1^2}}$$

При этом условие непрерывности ψ на границе соответствует условию непрерывности E_t, а условие непрерывности ψ'_x - условию непрерывности H_t. Плотность потока частиц соответствует плотности потока электромагнитной энергии (вектору Пойнтинга).

Оценим отличие n от 1:

$$\frac{2mU_0}{\hbar^2k_I^2}\approx\frac{2m\mu_g\,B}{4\pi^2\hbar^2}\lambda^2=\frac{e^2}{\hbar c}\frac{B}{e}\frac{\lambda^2}{4\pi^2}\approx2\cdot10^{-13}\ll1$$

Здесь было подставлено значение $\mu_{яд}=\frac{e\hbar}{2mc}$. Таким образом,

$$n\approx1\mp\frac{mU_0}{4\pi^2\hbar^2}\lambda^2$$

Это значение, очевидно, разное для разных значений проекции спина нейтрона на направление магнитного поля.

$$\begin{array}{lll}\text{Для} & m_s=\frac{1}{2} & n_+=1-\frac{1{,}91\mu_{яд}\,B\lambda^2}{4\pi^2\hbar^2}m.\\ \text{Для} & m_s=-\frac{1}{2} & n_-=1+\frac{1{,}91\mu_{я}\,B\lambda^2}{4\pi^2\hbar^2}m.\end{array}$$

Из закона преломления получим
или

$$\sin\psi_+=\frac{\sin\varphi}{n_+};\quad\sin\psi_-=\frac{\sin\varphi}{n_-}$$

$$\sin\psi_+-\sin\psi_-=\sin\varphi\frac{n_--n_+}{n_-n_+}$$

При разложении разности синусов двух близких углов появляются очевидные соотношения

$$|\psi_+-\psi_-|\ll\varphi;\quad\psi_++\psi_-\approx2\varphi;\quad n_+n_-\approx1$$

Окончательно

$$\theta=\Delta\psi=\psi_+-\psi_-=(n_--n_+)\,\mathrm{tg}\,\varphi=\frac{1,91\mu_s\,B\lambda^2}{2\pi^2\hbar^2}m\,\mathrm{tg}\,\varphi$$

Подстановка чисел дает $\theta\approx86\cdot10^{-6}$ рад $\approx3'$.

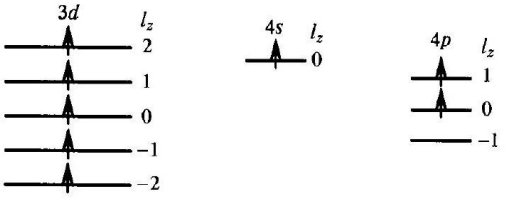


Рис. 162

6.

17: $\mathrm{H}-2; \mathrm{Li}-2; \mathrm{Fe}-1,3,5,7,9; \mathrm{Cl}-2,4,6,8; \mathrm{He}-1,3; \mathrm{Mg}$ - 1,3; $\mathrm{Hg}-1,3; \mathrm{U}-1,3,5,7$.

Решение. Рассмотрим в качестве примера атомы Fe и Cl . Электронная конфигурация атома железа представляет собой заполненные оболочки, как у Ar , сверх которых имеются 8 электронов $-3d^6 4s^2$. Максимально возможный спин атома $S = 1/2 \cdot 8 = 4$. Для этого один электрон из $3d$-оболочки и

один из $4s$-оболочки должны перейти в $4p$-оболочку (рис. 162). При этом мультиплетность $2S+1 = 2 \cdot 4 + 1 = 9$. Если из $4p$-оболочки один электрон вернется в $4s$ или $3d$-оболочку, то он обязан «перевернуть» спин, и общий спин уменьшится на 1 , и получим $2S + 1 = 2 \cdot 3 + 1 = 7$. Возврат второго электрона даст уменьшение еще на 1 , и получим $2S + 1 = 5$.

Шесть электронов в d-оболочке могут дать суммарный спин 2 , 1 и 0 . Получаются мультиплетности 5,3 и 1 (см. ответ).

У атома Cl электронная конфигурация $1s^2 2s^2 2p^5$. Максимальный спин $S = 7 \cdot 1/2 = 7/2$; мультиплетность $2S + 1 = 8$. Это достигается переходом одного электрона в $3s$-оболочку и двух - в $3p$-оболочку и т. д.

6.

18. $\mathrm{Sr}^{+} - 2; \mathrm{Li}^{+} - 1,3; \mathrm{Ca}^{+} - 2; \mathrm{C}^{2+} - 1,3; \mathrm{O}^{++} - 1,3$.

6.

19. 4.

6.

20. $\Delta\mathscr{E} = 2\pi\hbar c\left(\frac{1}{\lambda_1} - \frac{1}{\lambda_2}\right) \approx 2,1 \cdot 10^{-3} \ni$ В; $B = \frac{\Delta\mathscr{E}}{2\mu_{\mathrm{B}}} \approx 1,8 \cdot 10^5$Гс.

6.

21: $\Delta\mathscr{E}_B = \mu_{\mathrm{B}} B\left\{\frac{5}{3}; \frac{1}{3}; -1\right\}$ (три линии).

Решение. Для определения типа эффекта Зеемана (простой или сложный) необходимо сначала оценить величину спин-орбитального расщепления, пользуясь данными задачи,

$$\Delta U_{ls} = 2\pi\hbar c\left(\frac{1}{\lambda_{\mathrm{I}}} - \frac{1}{\lambda_2}\right) \approx \frac{2\pi\hbar c}{\lambda^2}\Delta\lambda \approx 2 \cdot 10^{-2} \ni \text{ В}$$

Далее оценим произведение $\mu_{\mathrm{b}} B \approx 2,9 \cdot 10^{-4}$ эВ. Сравнивая две полученные величины, мы видим, что $\mu_{\mathbf{5}} B \ll \Delta U_{ls}$, т. е. поле является слабым.

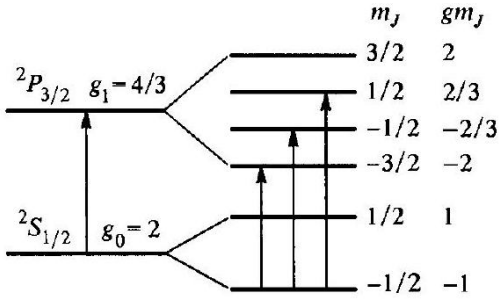


Рис. 163

Вычислим g-факторы состояний $^2P_{3/2}$ и $^2S_{1/2}$:

$$g_1 = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)} = \frac{3}{2} + \frac{\frac{1}{2}\cdot\frac{3}{2} - 1 \cdot 2}{2 \cdot \frac{3}{2} \cdot \frac{5}{2}} = \frac{4}{3}; \quad g_2 = 2 \quad (\text{ т. к. } L = 0)$$

Определим возможные переходы по формуле

$$\Delta\mathscr{E}_B = \mu_{\mathbf{E}} B\left(g_{\text{Кон}} m_J^{\text{кон}} - g_{\text{нач}}\, m_J^{\text{нач}}\right).$$

Однако в силу очень низкой температуры ($T = 0,5$ K) $kT \approx \approx 4 \cdot 10^{-5}$ В $\ll 2\mu_{\text{Е}}B$ (расщепление терма $^2S_{1/2}$). Таким образом, при этой

температуре заселен только нижний подуровень уровня $^2S_{1/2}\,(m_J = -1/2)$. Поэтому в спектре поглощения возможны только три линии (рис. 163):

$$\Delta\mathscr{E}_B = \mu_{\mathbf{G}}B \left\{ \begin{array}{l} \frac{2}{3} - (-1) = \frac{5}{3} \\ -\frac{2}{3} - (-1) = \frac{1}{3} \\ -2 - (-1) = -1 \end{array} \right.$$

6.

22. В спектре поглощения газа в магнитном поле будут наблюдаться шесть компонент расщепленной линии $^2P_{1/2} \to^2 D_{3/2}$. Это сложный эффект Зеемана ($\mu_{\mathbf{5}}B \ll U_{LS}; \mu_{\mathbf{6}}B \ll kT \approx 0,026$ эВ).

$$\frac{\Delta\mathscr{E}_B}{\mu_E B} = g_1 m_J^1 - g_2 m_J^2 = \left(\pm\frac{13}{15}; \pm\frac{11}{15}; \pm\frac{1}{15}\right).$$

6.

23. $2J + 1$.

6.

24. $\mathscr{E} = \mathscr{E}_0 + \mu_{\mathbf{5}}\text{Bgm}_J$, где $\mathscr{E}$ - энергия атома в магнитном поле, $\mathscr{E}_0$ без поля, $g = \frac{2J+1}{2L+1}$; а $J = \left\{ \begin{array}{l} L + 1/2 \\ L - 1/2 \end{array} \right.$, L-орбитальный момент валентного электрона, $m_J = -J, -J+1, ..., +J$.

6.

25. $\Delta\mathscr{E}_B = \mu_{\text{Е}}B\left(g_1 m_J^{(1)} - g_2 m_J^{(2)}\right) = \left\{\pm 1; \pm\frac{2}{7}; \pm\frac{39}{35}; \pm\frac{11}{7}; \pm\frac{6}{35}; \pm\frac{43}{45};\ \pm\frac{51}{35}; \pm\frac{2}{35}; \pm\frac{47}{35}\right\}\mu_{\text{Б}}\,B$ (18 линий).

6.

26. Это линии с $\Delta m_J = 0$ (колебания вдоль поля В не испытывают действие силы Лоренца). $\Delta\mathscr{S}_B = \left\{\pm\frac{2}{7}; \pm\frac{6}{35}; \pm\frac{2}{35}\right\} - 6$ линий. Такие линии называются л-линиями. Они видны при наблюдении поперек поля и не видны при наблюдении вдоль поля.

6.

27: Решение. Множитель Ланде

$$g = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

Для состояния $^2P_{3/2}(J = 3/2, L = 1, S = 1/2)$ этот множитель равен $g_1 = 4/3$; для состояния $^2S_{1/2}(J = 1/2, L = 0, S = 1/2), g_2 = 2$. Смещения расщепленных компонент мультиплета приведены в таблице:

$P_{3/2}$	m_J	$-3/2$	$-1/2$	$+1/2$	$+3/2$
	gm_J	-2	$-2/3$	$+2/3$	$+2$
$^2S_{1/2}$	m_J		$-1/2$	$+1/2$	
	gm_J		-1	$+1$	

Разрешенные переходы между компонентами мультиплетов (компонентами тонкой структуры) $^2P_{3/2}$ и $^2S_{1/2}$ удовлетворяют правилу отбора $\Delta m_J = m_J^{(1)} - m_J^{(2)} = 0, \pm 1$. Остальные переходы сильно подавлены. Разрешенные переходы и соответствующие им номера испускаемых спектральных линий с указанием поляризации (л или σ) приведены в таблице:

Переходы $m_j^{(1)} \to m_J^{(2)}$	Поляризация	$(gm_J)^{(1)} - (gm_J)^{(2)}$	№ линии
$-3/2 \to +1/2$	подавлен		
$-3/2 \to -1/2$	σ	$-2-(-1) = -1$	2
$-1/2 \to +1/2$	σ	$-2/3 - 1 = -5/3$	1
$-1/2 \to -1/2$	π	$-2/3 + 1 = 1/3$	4
$+1/2 \to +1/2$	π	$2/3 - 1 = -1/3$	3
$+1/2 \to -1/2$	σ	$2/3 + 1 = 5/3$	6
$3/2 \to +1/2$	σ	$2 - 1 = 1$	5
$3/2 \to -1/2$	подавлен		

Смещенные линии расположены симметрично относительно несмещенной: три линии смещены влево $(1, 2, 3)$, остальные три - вправо $(4, 5, 6)$. Всего получается шесть смещенных компонент.

Магнитное поле считается слабым, если ларморовская частота $\Omega = \mathrm{e}B/(2m_\mathrm{e}c)$ мала по сравнению с частотой $2\pi c\Delta\lambda/\lambda^2$. Это дает $B \ll \ll \left(4\pi m_\mathrm{e}c^2\Delta\lambda\right)/\left(e\lambda^2\right)$. В этом случае получается сложный эффект Зеемана. Для D-линии натрия должно быть $B \ll 3,7 \cdot 10^5$ Гс. В противоположном случае эффект Зеемана будет простым.

6.

28. $\Delta\mathscr{E}_B = \mu_\sigma B = \hbar\Omega = \hbar\frac{eB}{2mc}$; число уровней равно числу проекций $\mathbf{L}$ на B и равно $2L + \mathbf{1} = 7$.

6.

29. $\Delta\mathscr{E}_B = \mu_\mathbf{G} B\left(\Delta m_L + 2\Delta m_S\right) = \pm\mu_\mathbf{G} B, 0$, т. е. как и должно быть в сильном поле на три компоненты, поскольку для электродипольных переходов $\Delta m_S = 0, \Delta m_L = \pm 1, 0$ (правила отбора).

6.

30: $B = \frac{2\pi m_e c^2}{ed\Delta n}$.

Решение. Из трех линий спектра центральная несмещенная линия не пройдет, если пластинка для нее имеет толщину $m\lambda$.

Боковые линии пройдут, если для их длин волн λ' и λ'' толщина пластинки будет $m\lambda' + \lambda'/2$ и, соответственно, $m\lambda'' - \lambda''/2$. Таким образом, кристаллическая пластинка с заданным d и Δn (рис. 164) должна удовлетворять условию

$$d\Delta n = m\lambda = \left(m + \frac{1}{2}\right)\lambda' = \left(m - \frac{1}{2}\right)\lambda'',$$

где $\lambda' = \frac{2\pi c}{\omega+\Omega}$, а $\lambda'' = \frac{2\pi c}{\omega-\Omega}$ и ларморовская частота $\Omega = \frac{eB}{2m_e c}$. Отсюда

$$m + \frac{1}{2} = \frac{d\Delta n}{2\pi c}(\omega + \Omega); \quad m - \frac{1}{2} = \frac{d\Delta n}{2\pi c}(\omega - \Omega).$$

Вычитая эти равенства, получим

$$1 = \frac{d\Delta n}{2\pi c}2\Omega = \frac{d\Delta n}{2\pi c}\frac{eB}{2m_\mathrm{e}c},$$

откуда найдем искомое магнитное поле

$$B = \frac{2\pi m_e e^2}{\mathrm{e}d\Delta n}.$$

Ответ не зависит ни от длины волны исходной линии, ни от ориентации пластинки относительно поля (рис. 164).

6.

31. В сильном магнитном поле $\mathscr{E} = \mathscr{E}_0 + \mu_5 B\,(m_L + 2m_S)$. Уровень расщепится на 7 подуровней (рис. 165). Максимальная дополнительная энергия $\Delta U = 3\mu_5 B = 3,5 \cdot 10^{-4\text{эВ}}$.

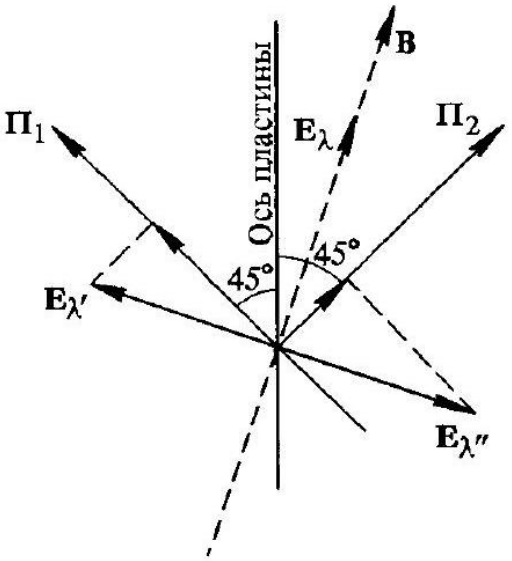


Рис. 164

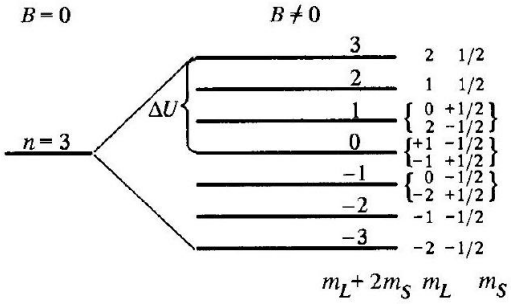


Рис. 165

6.

32. $L = \frac{4\pi m_e c^2}{eB} = 4,3$ cm.

6.

33. $L = \frac{hc}{2n\lambda\mu_5 B} = 2,8$ cm.

6.

34. Одна из линий дублета (переход ${}^2P_{3/2} \to {}^2S_{1/2}$) расщепляется в магнитном поле на 6 компонент $\left(\pm 1; \pm\frac{1}{3}; \pm\frac{5}{3}\right)\Omega$ с расстоянием между крайними компонентами

$$\Delta\omega = \frac{5}{3}\Omega - \left(-\frac{5}{3}\Omega\right) = \frac{10}{3}\Omega,$$

где $\Omega = eB/(2m_e c)$ - ларморовская частота. (Аналогично, но на 4 компоненты $\left(\pm\frac{2}{3}; \pm\frac{4}{3}\right)\Omega$, расщепляется вторая линия дублета - переход ${}^2P_{1/2} \to {}^2S_{1/2}$). Спектральный прибор для исследования расщепления должен не только разрешать расщепленные линии, но и не должен давать перекрытия порядков. Значит, область дисперсии $\Delta\lambda$ должна быть не меньше

$$\lambda\frac{\Delta\omega}{\omega} = \frac{\lambda^2}{2\pi c}\frac{10}{3}\frac{eB}{2m_e c} = \frac{5}{6}\frac{\lambda^2 eB}{\pi m_e c^2}.$$

Подставляя сюда $\Delta\lambda = \lambda/m$, где $m = d(n-1)/\lambda$ - порядок спектра, получим

$$d \leqslant \frac{6\pi m_c c^2}{5eB(n-1)} \approx 2,6 \text{ см}.$$

6.

39. $B \approx \frac{\pi\hbar c\Delta\lambda}{\mu_{\text{Б}}\lambda^2} \approx 3\kappa\text{Гс}$.

6.

40. $\frac{m_\mu}{m_e} = \left(\frac{3R_\infty}{4\cdot 2\pi\hbar\nu} - 1\right)^{-1} = 204,585$.

6.

41. $\Delta_{sl} \approx \frac{e^2\hbar^2}{2m_e^2c^2n^6r_1^3} ls\cos\hat{\mathbf{s}} \approx 0,91\cdot 10^{-17}$ эрг $\approx 0,57\cdot 10^{-5}{}_{\ni\text{В}}$.
$\Delta\mathscr{E}_{sl}$ можно найти приближенно. Для этого надо перейти в систему координат, связанную с электроном. В этой системе вращающийся протон создает магнитное поле $\mathbf{B}$, с которым и взаимодействует спиновой магнитный момент μ_s. Для оценки достаточно считать, что векторы $\mathbf{B}$ и $\boldsymbol{\mu}_{\text{s}}$ коллинеарны (точный расчет должен был бы учесть, что $\cos\hat{\mathbf{s}} \neq 1$). Укажем, что

$$\frac{(\mathbf{sl})}{r^3} = |\mathbf{s}|\cdot|1|\frac{\cos\mathbf{sl}}{n^6r_1^3}, \quad \text{где} \quad |\mathbf{s}| = s; \quad |\mathbf{1}| = l; \quad \cos\widehat{\mathbf{sl}} = \pm\mathbf{1}$$

Тогда

$$\Delta\S_{sl} \approx \frac{e^2\hbar^2}{2m_{\text{e}}^2c^2n^6r_1^3} ls\cos\hat{\mathbf{S}} \approx 0,91\cdot 10^{-17}\rho\Gamma \approx 0,57\cdot 10^{-5} \ni \text{ В}$$

При точном расчете

$$\Delta\mathscr{E}_{sl} = \frac{e^2\hbar^2}{4m_{\text{e}}^2c^2}\frac{1}{r_1^3}\frac{j_{\text{I}}(j_1+1) - j_2(j_2+1)}{n^3l\left(l+\frac{1}{2}\right)(l+1)} = \frac{\mu_{\text{B}}^2}{8r_1^3} = 4,53\cdot 10^{-5} \ni \text{ В}$$

где $n=2; l=1; j_1=3/2; j_2=1/2; s=1/2$, где r_1 - радиус первой боровской орбиты.
Отличие в 8 раз!

6.

42. $\Delta\lambda = 2\pi\hbar c\left(\frac{1}{10,2-\Delta_2} - \frac{1}{10,2+\Delta_1}\right) \approx \frac{hc}{(10,2)^2}(\Delta_1+\Delta_2) \approx 0,0004$, где 10,2 эВ - значение энергии кванта нерасщепленной первой линии серии Лаймана (переход $n=3\to n=1$); $\Delta_1 = \frac{1}{32}\frac{\mu_{\text{Б}}^2}{r_1^3}; \Delta_2 = \frac{2}{32}\frac{\mu_{\text{Б}}^2}{r_1^3}$.

6.

43. $\frac{\Delta\varrho_{Sl}|_{J+1,J}}{\Delta_{sl}|_{J,J-1}} = \frac{J+1}{J}$.

6.

44: Решение. Зеемановское расщепление должно быть больше доплеровского уширения за счет теплового движения атомов (в основном, водорода) и вращения звезды, т.е.

$$\frac{\Delta\omega}{\omega_0} = \frac{2\mu_\Sigma B}{\hbar\omega_0} \geqslant \left(\frac{\Delta\omega}{\omega_0}\right)_{\text{тепл}} + \left(\frac{\Delta\omega}{\omega_0}\right)_{\text{вращ}} = \frac{v_{\text{тепл}}}{c} + \frac{v_{\text{вращ}}}{c} \approx \frac{v_{\text{тепл}}}{c}.$$

Окончательно получим

$$B \geqslant \frac{\hbar\omega_0}{2\mu_{\mathrm{F}}c}\sqrt{\frac{2kT}{m_{\mathrm{p}}}} \approx 1,8\kappa\Gamma\mathrm{c}$$

6.

45. $B = \frac{Ry}{\mu_{\mathrm{G}}}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)\frac{1}{n_1+n_2-2} \approx \frac{Ry}{\mu_{\mathrm{G}}}\frac{1}{n^4} \approx 2,3\cdot 10^5\Gamma\mathrm{c}$, где $n \approx n_2 \approx n_1 = 10$.

6.

46. $\Delta\mathscr{E} \approx \frac{m_e c^2}{1024}\alpha^4 \approx 1,4\cdot 10^{-6}{}_{\text{эВ}}$.

6.

47. $(J+I) : (J+I-1) : (J+I-2) : \ldots$ - правило интервалов Ланде.

6.

48. $\lambda = \frac{2\pi\hbar c}{|\Delta\mathscr{E}_{\text{ст}}|} = 28,1$ см, где $\Delta\mathscr{E}_{\text{ст}} = 2g_{sp}g_s\frac{\mu_{\text{ядм}}\mu_{\text{Б}}}{r_{\text{Б}}^3}, g_s = 2$ - спиновый g-фактор электрона. Экспериментальное значение $\lambda = 21$ см. Этот результат получается и при теоретическом рассмотрении с учетом реального (неоднородного) распределения плотности спинового магнитного момента электрона.

Заметим однако, что для оценки величины сверхтонкого расщепления атомных состояний обычно считается, что это диполь-дипольное взаимодействие магнитных моментов электронов и ядра. В данной задаче это маг нитное взаимодействие электрона и протона, что приводит к оценке $\Delta\& = 2\frac{g_{\text{sp}}\,\mu_{\text{gд}}\,\mu_5}{r_6^3}$, и это соответствует длине волны перехода $\lambda \simeq 1$ м. Эта оценка достаточно сильно отличается от экспериментального значения $\lambda = 21$ cm. Ясно, что это обусловлено грубостью приближения, поскольку электронная орбита здесь считается классической. На самом деле электронная плотность «размазана» в объеме порядка $\frac{4}{3}\pi r_{\text{Б}}^3$. Если считать, как указано в условии, что электронная плотность однородна по объему шара радиусом $r_{\text{Б}}$, то модельная оценка и эксперимент отличаются намного меньше.

6.

49. $\Delta\mathscr{E}_{\text{сТ}} = \mathscr{E}_{\text{сТ}}(F=2) - \mathscr{E}_{\text{сТ}}(F=1) = 4g_j g_{s\text{p}}\frac{\mu_{\text{g}}\mu_{\text{E}}}{n^6 r_{\text{G}}^3} = 0,9\cdot 10^{-7}$ эВ, где $n = 2, g_j = \frac{4}{3}$ - фактор Ланде для электрона.

$\mathbf{F} = \mathbf{j} + \mathbf{s}_{\text{p}}, F = \left\{\begin{array}{l} 3/2+1/2=2 \\ 3/2-1/2=1 \end{array}\right.$ – это полный угловой момент атома.

6.

50. $\Delta\varrho_{\mathbf{H}} \approx 0,59\cdot 10^{-5}$ эВ. Радиус позитрония в $2p$-состоянии $r = 8r_1$, где r_1 - радиус боровской орбиты. Отношения частоты излучения позитрония к частоте излучения атомарного водорода

$$\frac{\nu_{\text{поз}}}{\nu_{\text{H}}} = \frac{m_{\text{p}}}{8^3\cdot 2,79 m_{\text{e}}} \approx 1,285, \quad \text{откуда} \quad \Delta\mathscr{E}_{\text{поз}} \approx 0,76\cdot 10^{-5}\ \text{В}$$

6.

51* Такое состояние невозможно. Если бы оно было возможно, то радиус электронной орбиты в таком «атоме» был бы много меньше компотоновской длины волны нейтрона.

Решение. При нерелятивистском рассмотрении полная энергия системы должна быть отрицательной:

$$\mathscr{E} = \frac{p^2}{2m_{\text{e}}} - \frac{\mu_{\text{e}}\mu_{\text{n}}}{r^3} < 0$$

Из соотношения неопределенностей $pr \sim \hbar$ выразим импульс электрона через r и подставим в предыдущее неравенство:

$$\mathscr{E} \approx \frac{\hbar^2}{2m_{\mathrm{e}}r^2} - \frac{\mu_{\mathrm{e}}\mu_{\mathrm{n}}}{r^3}$$

Радиус стационарной орбиты электрона оценим из минимума энергии $\frac{d\mathscr{E}}{dr} = 0$, откуда $r = \frac{3\mu_{\mathrm{e}}\mu_{\mathrm{n}}}{\hbar^2}m_{\mathrm{e}} \approx 8 \cdot 10^{-16}$ см $\ll \frac{\hbar}{m_{\mathrm{n}}c} \simeq 2 \cdot 10^{-14}$ см - комптоновской длины волны нейтрона. Последнее очевидное неравенство показывает неправомерность рассмотрения нейтрона в этой задаче как точечной частицы.

6.

52. $B = \frac{3\pi^2\hbar^2}{4\mu m d^2}$.

6.

53. $B \geqq \frac{m^2ce^3}{\hbar^3} \approx 10^9$Гс.

6.

54. $\mathcal{E} \approx \pm\frac{\mu^2}{r^3} \approx 3,2 \cdot 10^{-24}$ эрг $= 2 \cdot 10^{-12}$ эВ.

6.

55. $p_{\mathrm{ат}} = \frac{2\pi\hbar c}{\lambda E} \approx 4,3 \cdot 10^{-18}$ ед. СГСЭ; $l = \frac{p_{\mathrm{ат}}}{e} \approx 1$Å.

6.

56. Решение. Поскольку в сильных полях LS-связь разрывается, можно считать, что векторы **L** и **S** прецессируют вокруг вектора **B** независимо. Таким образом, сохраняющимися величинами являются L^2, S^2, L_z, S_z и

$$\langle U_{SL}\rangle = A\langle \mathbf{SL}\rangle = A\left\langle (L_xS_x + L_yS_y + L_zS_z)\right\rangle = A\left\langle (L_zS_z)\right\rangle = Am_Lm_S$$

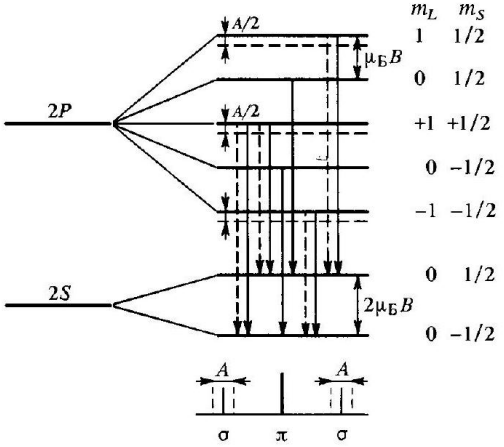


Рис. 167

Расщепление линий показано штрихами на рис. 167. В спектре излучения л-линия не расщепляется (у нее $m_L = 0$), а б-линии становятся дублетами, раздвинутыми на величину $A/\hbar\left[\mathrm{c}^{-1}\right]$. Экспериментально эффект наблюдался на Li .

6.

57. $g = 0,34; \mu = g\mu_{\text{яд}}\, I = 0,85\mu_{\text{яд}}$.

6.

58. Сигнал в магнитном поле пропорционален разности заселенности подуровней $\Delta n \approx N\frac{\mu B}{kT}$. Увеличение сигнала $a = \frac{A_0}{A_1} = \frac{\Delta n_0}{\Delta n_1} \approx \frac{B_0}{B} = 100$.

6.

59. Сигнал в резонансе $\propto (h\nu)^2_{\text{рез}}\, \frac{N_0}{kT} \propto \nu^2$, т. е. увеличится в четыре раза.

6.

60. $T_{\min} \approx \frac{h^2\nu^2 I^2}{B^2 k d^3} \approx 0,6 \cdot 10^{-7}$ K.

Решение. В методе адиабатического размагничивания поле B переводит решетку в парамагнитное состояние, в котором магнитные моменты ядер ориентируются по полю B. При этом $kT_{\text{нач}} \ll \mu_{\text{яд}}\, B$. При снятии внешнего поля происходит разупорядочение системы и понижение ее температуры. Выделившееся тепло отводится, и процесс можно повторить. При полном разупорядочении можно получить $T \approx 0$ K. Однако этого не происходит, поскольку есть взаимодействие, приводящее систему к установлению антиферромагнитного упорядочения. В принципе наличие энергии взаимодействия любой природы устанавливает предел на минимально достижимую темнературу $T_{\min}$, определяемую условием

$$kT_{\min} \approx \mathscr{E}_{\text{В3}}$$

Установление антиферромагнитного упорядочения в цепочке ядер ^{63}Cu (рис. 168) происходит за

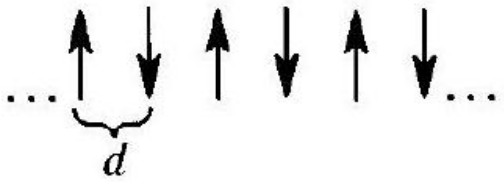


Рис. 168 счет магнитного (диполь-дипольного) взаимодействия атомов. В приближении ближайших соседей энергия взаимодействия $\mathscr{E}_{\text{вз}} = \mu^2/d^3$. Из условия на ядерный магнитный резонанс следует, что магнитный момент ядра $^{63}\text{Cu}\mu = g_I\mu_{\text{яд}}\, I$, где $g_I = \frac{h\nu}{\mu_{\text{яд}}\, B}$, откуда энергия взаимодействия атомов

$$\mathscr{E}_{\text{В3}} = \frac{g_I^2\mu_{\text{g}\mu}^2 I}{d^3} = \left(\frac{h\nu I}{B}\right)^2 \frac{1}{d^3}$$

а также

$$T_{\min} = \left(\frac{h\nu I}{B}\right)^2 \frac{1}{kd^3} \approx 0,6 \cdot 10^{-7} \text{ K}$$

6.

61* $v_{\text{рез}} = 1,6\text{ГГ}$.

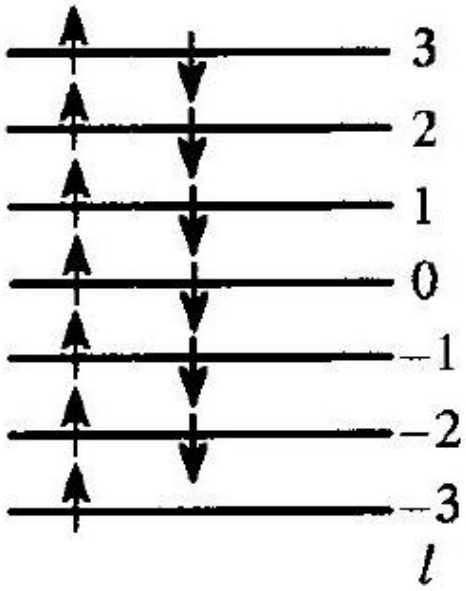


Рис. 169

Решение. Поскольку электронные оболочки $5s$ и $5p$ полностью заполнены, то парамагнитные свойства иона определяются 13 электронами незаполненной $4f$-оболочки. В соответствии с первым правилом Хунда эти электроны располагаются так, чтобы образовать максимальный спин $S_{\max}$, и при данном $S_{\max}$ - максимальный орбитальный момент $L_{\max}$ (рис. 169). На f-оболочке ($l = 3$) имеется $2(2l + 1) = 14$ мест, тринадцать из которых заняты. Поскольку в квантовой физике за велечину момента принимают значение его максимальной проекции на заданную ось (в един ницах $\hbar$), то

$$(S_z)_{\max} = \frac{1}{2}; \quad (L_z)_{\max} = 3 + 2 + 1 + 0 - 1 - 2 = 3$$

В соответствии со вторым правилом Хунда

$$J = L + S = 3 + \frac{1}{2} = \frac{7}{2}.$$

Вычислим g-фактор

$$g = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)} = \frac{8}{7}.$$

Резонансную частоту ЭПР найдем по формуле

$$v_{\text{рез}} = \frac{g\mu_{\text{E}}B}{h} = 1,6\text{ГГ}_{\text{L}}.$$

6.

62. $v = 1,12\text{ГГ}(S = 1; L = 5; J = 4; g = 4/5)$.

6.

63. $M_0 = \frac{N_{\text{A}}\rho h\nu}{B_{\text{рез}}\,A} = 2980$ Гс, где A - атомная масса Dy .

6.

64. $M_0 = \frac{N_{\text{A}}\rho}{A} g\mu_{\mathbf{6}} J = 2723$ Гс, где A - атомная масса эрбия Er , $v = \frac{g\mu B}{h} \approx 1,68$ ГГц, где $g = 6/5$.

6.

65. Для полученной конфигурации атома $S_{\max} = 3/2, \quad L_Z^{\max} = 2$, $J = 1/2$, т. е. состояние $^4D_{1/2}$. При этом $g = 0$, что означает, что $\boldsymbol{\mu}_{\text{сумм}} \perp \mathbf{J}$. Таким образом $\mu_{\text{J}} = 0$, а значит, пучок не расщепится.

6.

66.

$$\mu = \frac{LkT}{B\hbar N_{\text{A}}} = 2,62\mu_{\text{яД}} = 13,25 \cdot 10^{-24} \text{ эрг /Гс.}$$

Решение. Молярная масса тефлона $n \cdot 50$ г/моль, поэтому образец тефлона массой 50 г содержит $1/n$ молей тефлона. В этом образце в соответствии с химической формулой содержится $N_0 = 2N_{\text{A}} n\frac{1}{n} = 2N_{\text{A}}$ атомов фтора. На

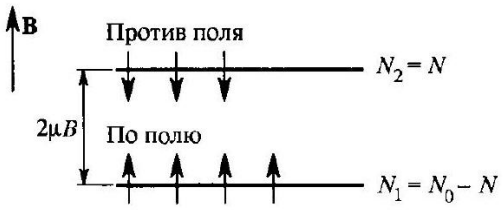


Рис. 170 рис. 170 изображена схема расщепления уровней ядра фтора в магнитом поле. Так как спин ядра равен 1/2, то получается двухуровневая система. Из полного числа N_0 ядер на верхнем уровне находятся N_2 ядер фтора. Пусть $N_2 = N$. На нижнем уровне остается $N_1 = N_0 - N$ ядер. Разность $\Delta N = N_1 - N_2 = N_0 - 2N$. В соответствии с распределением Больцмана

$$\frac{N_2}{N_1} = \frac{N}{N_0 - N} = \exp\left(-\frac{\Delta\mathscr{E}}{kT}\right),$$

где $\Delta\mathscr{E} = 2\mu B, \mu$ - магнитный момент ядер фтора.
Из этого следует

$$N = \frac{N_0 \exp(-\Delta\mathscr{E}/kT)}{1 + \exp(-\Delta\delta/kT)}$$

$$\Delta N = N_0 - 2N = N_0 \frac{1 - \exp\left(-\frac{\Delta\delta}{kT}\right)}{1 + \exp\left(-\frac{\Delta\varepsilon}{kT}\right)} \approx N_0 \frac{\frac{\mu B}{kT}}{1 - \frac{\mu B}{kT}} \approx \frac{\mu B}{kT} N_0.$$

Здесь мы учли, что $\frac{\mu_{\text{яд}} B}{kT} = 1,4 \cdot 10^{-6} \ll 1$ и поэтому разложим экспоненты в ряд. При снятии поля половина ядер из ΔN разориентируется, т. е. образец получит момент импульса

$$L = \frac{\Delta N}{2}\hbar = \frac{1}{2}\frac{\mu B\hbar}{kT} N_0 = \frac{\mu B\hbar N_{\text{A}}}{kT}$$

откуда и определим магнитный момент ядра фтора

$$\mu = \frac{LkT}{B\hbar N_{\text{A}}} = 13,25 \cdot 10^{-24} \ni \text{ г/Гс} = 2,62\mu_{\text{яд}}$$

где $\mu_{\text{яд}} = 5,05 \cdot 10^{-24}$ эрг/Гс - ядерный магнетон Бора. При написании этой формулы мы учли, что магнитный момент ядра $^{19}_{9}$ F определяется неспаренным протоном, находящемся в состоянии $2s_{1/2}$ (это один протон сверх заполненной оболочки из 8 протонов). Поскольку в этом состоянии орбитальный момент $l = 0$, то у этого протона угловой момент является чисто спиновым и равен $\hbar/2$. При перевороте спина угловой момент изменяется на $\hbar$.

6.

67. $B > \frac{\Delta\varepsilon}{2\mu} = 1,7 \cdot 10^9$Гс.

6.

68* $\alpha \approx 3 \cdot 10^{-6}$.

Решение. В магнитном поле атомы водорода поляризуются из-за того, что проекция их магнитного момента на направление поля принимает два значения

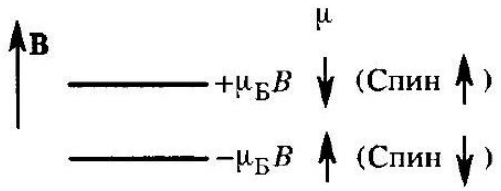


Рис. 171 $\pm\mu_{\text{Б}}$. Как в любой двухуровневой системе, полное число атомов $N_0 = N_\uparrow + N_\downarrow$. Отношение числа атомов H со спином по полю $N\uparrow$ к числу атомов со спином против поля $N\downarrow$ (рис. 171).

отсюда

$$\frac{N_\downarrow}{N_\uparrow} = \exp\left(-\frac{2\mu B}{kT}\right)$$

$$N_\uparrow = \frac{N_0}{1+\exp\left(-\frac{2\mu_{\text{E}}B}{kT}\right)}; \quad N_\downarrow = \frac{N_0 \exp\left(-\frac{2\mu_{\text{E}}B}{kT}\right)}{1+\exp\left(-\frac{2\mu_{\text{E}}B}{kT}\right)}$$

Поскольку $N_\downarrow < N_\uparrow$, то число атомов с антипараллельными спинами равно $2N_\downarrow$, а их относительное число

$$\alpha = \frac{2N_\downarrow}{N_0} = \frac{2\exp\left[-2\mu_{\text{E}}B/(kT)\right]}{1+\exp\left[-2\mu_{\text{E}}B/(kT)\right]} \approx 2\exp\left(-\frac{2\mu_\Sigma B}{kT}\right) \approx 3\cdot 10^{-6}.$$

6.

69: $T_{\max} \approx \frac{\mu_{\text{E}}^2}{ka^3} \approx 2\cdot 10^{-2}$ K.

Решение. См. также задачу 6.60. Нагревание всегда разупорядочивает структуру. Поэтому $kT_{\max} \approx \mathscr{E}_{\text{вз}}$. Энергия магнитного взаимодействия атомов $\mathscr{E}_{\text{вз}} \approx \mu^2/a^3$. Для оценки магнитного момента атома разумно взять магнетон Бора, поскольку электронный магнитный момент $\mu \lesssim \mu_{\text{б}}$. Отсюда $T_{\max} \approx \mu_{\text{B}}^2/\left(ka^3\right) \approx 2\cdot 10^{-2}$ K.

Эта оценка ясно показывает, что чисто магнитно-дипольное взаимодействие не может объяснить наблюдаемую величину температуры Кюри ферромагнетиков $T_{\text{K}} \sim 10 \div 1000$ K. Магнитное упорядочение у ферромагнетиков имеет другую природу - обменное взаимодействие, которое по своей сути является электростатическим (см. задачу 6.78). Величина электростатического взаимодействия двух электронов, находящихся на расстоянии a порядка e^2/a, что соответствует температуре упорядочения $T \sim e^2/(ka) \simeq 5\cdot 10^4$ K. Т.к. обменное взаимодействие составляет обычно $(0,01 \div 0,1)$ долю электростатического, то видно что это обеспечивает наблюдаемые T_{K} практически всех материалов.

6.

70: $\mathscr{E}_n = \hbar\omega_c\left(n+\frac{1}{2}\right)$, где $n = 0,1,2,...; \omega_c = \frac{eB}{m_e c}$ - циклотронная частота; $\mathscr{E}_0 = 5,8\cdot 10^{-6}$ эВ.

Решение. В магнитном поле электрон движется по окружности с циклотронной частатой $\omega_c = \frac{eB}{mc}$. Такое движение можно описать изменением только одной координаты - угла поворота. Тем самым задача сводится к задаче об одномерном осцилляторе с законом квантования $\mathscr{E}_n = \hbar\omega_c(n+1/2)$.

Покажем как это можно получить используя уравнения Гамильтона. В магнитном поле соотношение между импульсом $\mathbf{p}$ и скоростью $\mathbf{v}$ частицы не имеет привычной формы $\mathbf{p} = m\mathbf{v}$. Соотношение между $\mathbf{p}$ и $\mathbf{v}$ в присутствии магнитного поля можно получить двумя способами. Первый из них состоит в том, что когда частица из области $B = 0$ попадает в область $B \neq 0$ (либо B как-либо меняется от нуля до B_0), то возникает вихревое электрическое поле E. Согласно уравнению Максвелла

$$\operatorname{rot}\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t} = -\frac{1}{c}\frac{\partial}{\partial t}\operatorname{rot}\mathbf{A}$$

откуда следует, что $\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}$. За время возникновения поля оно меняет скорость частицы

$$m\frac{d\mathbf{v}}{dt} = q\mathbf{E} = -\frac{q}{c}\frac{\partial\mathbf{A}}{\partial t}$$

откуда инегрированием получаем

$$m\mathbf{v} = \mathbf{p}_0 - \frac{q}{c}\int \frac{\partial \mathbf{A}}{\partial t}dt = \mathbf{p}_0 - \frac{q}{c}\mathbf{A}$$

Отсюда следует, что $m\mathbf{v} + \frac{q}{c}\mathbf{A} = \text{const}$, и эта константа не зависит от на личия поля. Эту константу можно рассматривать как эффективный импульс $\mathbf{p} = m\mathbf{v} + \frac{q}{c}\mathbf{A}$. Для электрона ($q = -e$) $\mathbf{p} = m\mathbf{v} - \frac{e}{c}\mathbf{A}$.

Второй способ состоит в том, что полный импульс заряженной частицы складывается из двух частей $\mathbf{p} = \mathbf{p}_{\text{кин}} + \mathbf{p}_{\text{пол}}$, где $\mathbf{p}_{\text{кин}} = m\mathbf{v}$, а $\mathbf{p}_{\text{пол}}$ - им пульс электромагнитного поля, образованного электрическим (кулоновским) полем частицы и постоянным магнитным полем внешних источников.

$$\mathbf{p}_{\text{пол}} = \frac{1}{4\pi c}\int [\mathbf{EB}]dV, \quad \text{где} \quad \operatorname{div}\mathbf{E}(\mathbf{r}) = 4\pi\rho = 4\pi q\delta(\mathbf{r} - \mathbf{r}')$$

$\mathbf{r}$ - положение частицы (при $v \ll$ ее можно считать покоящейся и не учитывать магнитного поля, создаваемого ею самой). Поскольку $\mathbf{B} = \operatorname{rot}\mathbf{A}$, то можно показать, что в этих предположениях $\mathbf{p}_{\text{пол}} = \frac{q}{c}\mathbf{A}$, т. е. $\mathbf{p} = m\mathbf{v} + \frac{q}{c}\mathbf{A}$.

Энергия частицы в постоянном магнитном поле есть чисто кинетическая (без учета спина), поэтому гамильтониан

$$\mathcal{H} = \frac{mv^2}{2} = \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2 = \frac{1}{2m}\left[p_x^2 + (p_y - m\omega_c x)^2 + p_z^2\right]$$

где $\omega_c = \frac{qB}{mc}$ - циклотронная частота. Мы рассматриваем общий случай $p_z \neq 0$. Классические уравнения движения Гамильтона

дают

$$\dot{\mathbf{r}} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}}; \quad \dot{\mathbf{p}} = -\frac{\partial \mathcal{H}}{\partial \mathbf{r}}$$

$$\begin{cases} \dot{x} = \frac{p_x}{m} \\ \dot{y} = \frac{p_y - m\omega_c x}{m}, \\ \dot{z} = \frac{p_z}{m}, \end{cases} \qquad \text{а также} \qquad \begin{cases} \dot{p}_x = -(p_y - m\omega_c x)\,\omega_c \\ \dot{p}_y = 0 \\ \dot{p}_z = 0 \end{cases}$$

Видно, что p_y и p_z являются интегралами движения, а $\dot{y}$ - не является интегралом движения. Это есть проявление того факта, что в магнитном поле $B_0 \| OZx$ - и y-компоненты скорости частицы не могут иметь одновременно определенных соотношений. Обозначим $p_y = p_{y0} = \text{const}; p_z = p_{z0} = \text{const}$. Поскольку по условию задачи $\mathbf{v} \perp \mathbf{B}$, то $p_{z0} = 0$.

Тогда $\mathcal{H} = \frac{1}{2m}\left[p_x^2 + (p_{y0} - m\omega_c x)^2\right]$.

Сделаем замену переменных $x' = x + \frac{p_{y0}}{m\omega_c}$. Тогда $p_x = p'_x$ и

$$\mathscr{H} = \frac{1}{2m}p_x^{2\prime} + \frac{m\omega_c^2}{2}x'^2$$

Мы свели таким образом гамильтониан частицы к гамильтониану одномерного гармонического осциллятора. Воспользовавшись результатами квантово-механической задачи о квантовом осцилляторе, запишем по аналогии энергию уровней, называемых уровнями Ландау:

$$\mathscr{E}_n = \hbar\omega_c\left(n + \frac{1}{2}\right)$$

Это - система эквидистантных уровней. Каждый уровень имеет бесконечную кратность вырождения, т. к. энергия не зависит от $p_y, -\infty < p_y < +\infty$. При этом координата положения равновесия осциллятора $x' = 0$, т. е. $x = -\frac{p_{y0}}{m\omega_c}$ - не определена.

Минимальная энергия электрона $\hbar\omega_c/2 = 5,8 \cdot 10^{-6}$ эВ. Учет спина электрона приводит к добавке $(\boldsymbol{\mu}\mathbf{B})$ в энергию и спиновому расщеплению уров-

ней $2m_s\mu_{\mathbf{5}}B, (m_s = \pm 1/2)$. Для свободного электрона $\mu_{\mathbf{D}}B = \hbar\omega_c/2$. На рис. 172 изображено расщепление уровней. Стрелками изображено направление магнитных моментов электрона. Низшее состояние определяется тем, что $\boldsymbol{\mu}\|\mathbf{B}$. При этом спин $\mathbf{S}$ антипараллелен полю $\mathbf{B}$.

6.

71: $S^{\text{p}}_{\min} = \frac{\pi\hbar eB}{c} \approx 1,66 \cdot 10^{-43}$ эрг $\cdot\Gamma$; $S^{\mathbf{R}}_{\min} = \frac{\pi\hbar c}{eB} = 6,56 \cdot 10^{-11}$ см^2.

Решение. Условие вращения электрона в магнитном поле по окружности

$$\frac{mv_\perp^2}{R} = \frac{e}{c}v_\perp B$$

дает в координатном пространстве (R-пространстве) радиус ларморовского кружка

$$R = \frac{mc}{eB} v_\perp$$

Преобразуем это выражение:

$$R^2 = \left(\frac{mc}{eB}\right)^2 v_\perp^2 = \frac{2mc^2}{e^2B^2}\frac{mv_\perp^2}{2} = \frac{2mc^2}{e^2B^2}\mathscr{E}_\perp$$

где $\mathscr{E}_\perp$ - кинетическая энергия поперечного движения частицы. Так как $\mathscr{E}_\perp$ квантуется, т. е. $\mathscr{E}_\perp = \hbar\omega_c\left(n+\frac{1}{2}\right)$, то квантуется и квадрат радиуса орбиты, т. е. площадь

$$S_n = \pi R_n^2 = 2\pi\frac{mc^2}{e^2B^2}\hbar\omega_c\left(n+\frac{1}{2}\right)$$

Запишем далее уравнение движения (**R** - это проекция **r** на плоскость, перпендикулярную B)

$$m\frac{d\mathbf{v}}{dt} = \frac{e}{c}[\mathbf{vB}], \quad \mathbf{v} = \frac{d\mathbf{r}}{dt}, \quad \text{т. е.} \quad \frac{d\mathbf{v}}{dt} = \frac{e}{mc}\left[\frac{d\mathbf{r}}{dt}, \mathbf{B}\right].$$

Интегрируя и отбрасывая постоянную интегрирования, получаем

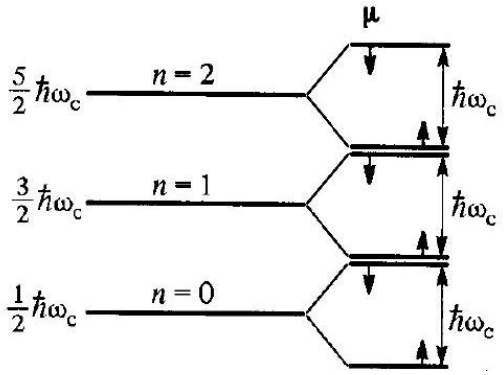


Рис. 172

$\mathbf{v} = \frac{e}{mc}[\mathbf{rB}]$. Поскольку $\mathbf{v} \perp \mathbf{B}$ и $\mathbf{r} \perp \mathbf{B}$, то $\mathbf{v}_\perp = \frac{eB}{mc}[\mathbf{R}, \mathbf{z}]$.

Отсюда видно, что в импульсном пространстве (или пространстве скоростей) траектория получается умножением на $eB/(mc)$ и ее поворотом на 90° вправо (по часовой стрелке), если смотреть с конца вектора B.

Таким образом, траектория электрона в пространстве скоростей - тоже окружность и

$$S_n^v = \pi v_\perp^2 = \pi R_n^2\left(\frac{eB}{mc}\right)^2 = 2\pi\frac{\hbar\omega_c}{m}\left(n+\frac{1}{2}\right)$$

Минимальная площадь $S_0^v = \frac{\pi\hbar\omega_c}{m}$, или, в импульсном пространстве,

$$S_{\min}^{\text{p}} = S_0^p = m^2v_\perp^2\pi = \pi m\hbar\omega_{\text{c}} = \frac{\pi\hbar eB}{c} = 1,66\cdot10^{-43} \ni \text{р}\Gamma\cdot\Gamma.$$

Минимальная площадь в **R**-пространстве

$$S_{\min}^{\mathbf{R}} = \pi\frac{mc^2}{e^2B^2}\hbar\omega_c = \frac{\pi\hbar c}{eB} = 6,56\cdot10^{-11}\ \text{см}^2$$

Заметим, что из квантования площади в **R**-пространстве следует квантование магнитного потока, пронизывающего орбиту электрона,

$$\Phi_n = \pi R_n^2 B = \Phi_0\left(n+\frac{1}{2}\right)$$

где $\Phi_0 = \frac{2\pi\hbar c}{e} = \frac{2\pi e}{\alpha}$, где α - постоянная тонкой структуры, а Φ_0 - минимальный магнитный поток (квант магнитного потока).

6.

72: $R = \frac{\gamma M}{c^2 \ln(m_e c^2/\mathscr{E}_2)} \approx 7$ км; $B = \frac{\mathscr{E}_1 m_e c^2}{2\mu_\text{b} \varepsilon_2} = 4,77 \cdot 10^{12}$Гс.

Решение. Вблизи нейтронной звезды находится другая звезда (красный гигант), образующая с нейтронной звездой двойную систему. За счет сильного гравитационного поля происходит аккреция, т. е. захват протонноэлектронной плазмы красного гиганта и ее падение на нейтронную звезду. При этом непрерывное (тормозное) рентгеновское излучение уносит выделившуюся кинетическую энергию.

Магнитное поле у нейтронной звезды возникает в силу сохранения магнитного потока из первоначального поля звезды и ее «раскрутки». Предполагается, что исходной была звезда типа Солнца. На поверхности звезды «аннигиляционный» γ-квант имеет энергию, равную $m_\text{e}c^2 = 511$ кэВ. После «преодоления» гравитационного поля он «краснеет» (см. задачу 1.4) и на поверхности Земли имеет энергию $\mathscr{E}_2 = 460$ кэВ. Таким образом,

$$\ln \frac{m_e c^2}{\mathscr{E}_2} = \frac{\gamma M}{c^2 R},$$

откуда следует ответ

$$R = \frac{\gamma M}{c^2 \ln\left(m_\text{e} c^2/\mathscr{E}_2\right)} \approx 7 \text{ км} .$$

В магнитном поле уровни энергии свободного электрона (уровни Ландау) $_n = \hbar\omega_\text{c} n = 2\mu_\mathbf{5} B n$. Как и в первом случае, это излучение преодолевает гравитационное поле нейтронной звезды и на поверхности Земли имеет энергию $\mathscr{E}_1 = 50$ кэВ. Таким образом,

$$\ln \frac{2\mu_\sigma B}{\mathscr{E}_1} = \frac{\gamma M}{c^2 R}, \text{ откуда искомое поле } B = \frac{\mathscr{E}_1 m_\text{e} c^2}{2\mu_\Sigma \mathscr{E}_2} = 4,77 \cdot 10^{12}\text{Гс}.$$

6.

73* $P = 0,3$.

Решение. В силу несохранения четности при β-распаде число электронов, вылетевших по и против спина ядра, будет различным. Но если число ядер со спином вверх и вниз будет одинаковым, то результирующая асимметрия вылета исчезнет, и эффект несохранения четности не проявится. Поэтому необходимо иметь преимущественную поляризацию ядер, что достигается в магнитном поле при низких температурах.

В магнитном поле уровень ядра с $I = 1$ расщепляется на три подуровня, соответствующие значениям магнитного квантового числа $m_I = 1, 0, -1$ и расстояние между ними $\Delta\mathscr{E} = g\mu_\text{яд} H$. Отношение заселенностей подуровней равно:

$$\frac{N(m_1)}{N(m_2)} = \exp\left[\frac{(m_1 - m_2)\, g\mu_\text{gp}\, B}{kT}\right] = e^\alpha, \text{ где } m_1 = +1, m_2 = -1$$

Искомая поляризация ядер

$$P = \frac{e^a - 1}{e^a + 1} = 0,3$$

Это означает, что только 30% распадов дадут асимметричный эффект, который наблюдается на симметричном фоне распадов остальных ядер.

6.

74* $n = 2, l = 1$, число поду ровней 5 .

Решение. Главное квантовое число $n = \sqrt{\frac{\text{Ry}}{\varrho}} = 2$. При этом $n = n_r + l + 1$, где радиальное квантовое число n_r определяет число нулей радиальной части волновой функции на $(0, \infty)$, т. е. $n_r = 0$. Отсюда следует, что $l = 1$, и мы имеем $2p$-состояние. Число подуровней равно 5 $(m_l + 2m_s = \pm 2; \pm 1; 0)$.

6.

75. $2s$-состояние $(l = 0)$; $2s + 1 = 2$ - число подуровней. Оно не зависит от величины поля $\mathbf{B}$, т. к. данный уровень - синглет.

6.

76. $\lambda = \frac{2\lambda_1\lambda_2}{\lambda_1-\lambda_2} = 1034571,4\text{Å} \approx 0,01$ cm.

Решение. В схеме Рассела-Саундерса снятие вырождения и расщегт ления терма ^3P по величине полного момента $\mathbf{J}$ с образованием подуровней тонкой структуры $^3P_2, ^3P_1, ^3P_0$ есть результат спин-орбитального взаимодействия. Энергия подуровней отличается от энергии терма на величину энергии спин-орбитального взаимодействия

$$\mathfrak{E}_{LS} = A((\mathbf{LS})\rangle = \frac{1}{2}\left\langle \mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right\rangle = \frac{A}{2}[J(J+1) - L(L+1) - S(S+1)]$$

При этом

$$\mathscr{E}\left(^3P_2\right) - \mathscr{E}\left(^3P_1\right) = \left[\mathscr{E}\left(^3P\right) + \mathscr{E}_{LS}(J=2)\right] - \left[\mathscr{E}\left(^3P\right) + \mathscr{E}_{LS}(J=1)\right] = 2A > 0$$

Знак константы спин-орбитального взаимодействия однозначно связан с правилом Хунда: если занято меньше половины свободных мест, то ниже по энергии лежит состояние с меньшим J и получается т. н. нормальный мультиплет. Действительно, электронная конфигурация $O^{2+} : 1s^2 2s^2 2p^2$ и в незаполненной L-оболочке, содержащей $2(2l+1) = 6$ мест, занято всего 2 места. Аналогично

$$\mathscr{E}\left(^3P_1\right) - \mathscr{E}\left(^3P_0\right) = \left[\mathscr{E}\left(^3P\right) + \mathscr{E}_{LS}(J=1)\right] - \left[\mathscr{E}\left(^3P\right) + \mathscr{E}_{LS}(J=0)\right] = A$$

Согласно правилам Бора

$$\mathscr{E}\left(^3P_2\right) - \mathscr{E}\left(^3P_1\right) = \left[\mathscr{E}\left(^1D_2\right) - \frac{hc}{\lambda_1}\right] - \left[\mathscr{E}\left(^1D_2\right) - \frac{hc}{\lambda_2}\right] = hc\left(\frac{1}{\lambda_2} - \frac{1}{\lambda_1}\right)$$

Аналогично

$$\mathscr{E}\left(^3P_1\right) - \mathscr{E}\left(^3P_0\right) = \frac{hc}{\lambda} = \frac{1}{2}\left(\mathscr{E}\left(^3P_2\right) - \mathscr{E}\left(^3P_1\right)\right) = \frac{hc}{2}\left(\frac{1}{\lambda_2} - \frac{1}{\lambda_1}\right).$$

Откуда получаем ответ:

$$\lambda = \frac{2\lambda_1\lambda_2}{\lambda_1 - \lambda_2} = 1034571,4\text{Å} \approx 0,01 \text{ cm}.$$

6.

77. $\lambda = \frac{2\lambda_1\lambda_2}{\lambda_2-\lambda_1} = 15784$Å (см. решение задачи 6.76. Однако здесь получается обращенный мультиплет (т. к. число электронов в незаполненной L-оболочке равно 4), когда большей энергии соответствует меньшее J: состояние $^3P_1$ лежит выше по энергии состояния $^3P_2$).

6.

78. $A = 0,4$ В; $\mathscr{E}_\text{k} = +9,2$ эВ.

Заметим, что энергия возбужденного состояния атома гелия $\mathscr{E}_\text{пара} = -W_\text{пара} = \mathscr{E} + \mathscr{E}_\mathbf{K} + A$, а $\mathscr{E}_\text{орто} = -W_\text{орто} = \mathscr{E} + \mathscr{E}_\mathbf{K} - A$, т. к. энергия обменного взаимодействия $V = -A(S(S+1)-1) = \begin{cases} -A \text{ для ортогелия,} \\ +A \text{ для парагелия,} \end{cases}$ а энергия электронной конфигурации $1s^1 2s^1$ равна $\mathscr{E} = -68$ эВ .

6.

79. $v_{\text{ре з}} = \frac{2\mu_\Sigma B}{h} = 18,7\Gamma\Gamma_\text{L}$.

6.

80. $L = 6$.

18.2 Nuclear and Particle Physics

18.2.1 General questions about nuclei and radioactivity

ФР.МФТИ-кр. Радиус Чармония по двум уровням (!?!?!??)

Известно, что есть частица Чармоний из - и $\bar{c}$-кварка. Известно, что у него энергия основного состояния $E_0 = 3$ГэВ, а энергия первого возбужденного состояния $E_1 = 3.7$ГэВ. Оценить характерный радиус чармония.

Указание: считать, что при сильном взаимодействии энергию можно оценить как $E = mc^2 - \frac{q^2}{2m}$, где q - цветовой заряд (по модулю) обоих частиц.

Solution

(в 2 строчки решается задача, лень писать даже)

Об адекватности и содержательности задачи.

Как вообще узнать, какой первый возбужденный уровень частицы, которая скорее всего за доли секунды распадается?

Применима ли вообще квантовая механика???

Короче, тут предполагается тупо использовать детскую аппроксимацию и скорее всего авторы вообще ничего про сильные взаимодействия не знают, и из вуза их нужно уволить.

18.2.2 Problems about radioactivity 1

О3.1-7.1

Определить среднюю плотность ядерного вещества, полагая, что радиус ядра равен $R = 1,3A^{1/3}$, где A - массовое число (число нук.1онов). Энергия связи на один нуклон $B = 8,5$МВ/ нуклон. Средняя масса нуклона $m_{\text{N}} \approx 940\text{МВ}/c^2$.1)

7.

1. $\rho = \frac{m_{\text{N}}A - BA/c^2}{4\pi R^3/3} = 1,8 \cdot 10^{14}\Gamma/\text{см}^3$.

О3.1-7.2

Определить Энергию $\mathscr{E}_{\text{k}}$ кулоновского расталкивания протонов в ядре в предположении, что протоны распределены по ядру равномерно. Установить зависимость $\mathscr{E}_{\text{k}}$ от числа нуклонов и заряда ядра Z. Радиус ядра $R = 1,3A^{1/3}$ фм.

7.

2. $\mathscr{E}_{\mathbf{K}} \approx \frac{3}{5}\frac{Z^2e^2}{R} \approx 0,66Z^2A^{-1/3}$ [МэВ].

О3.1-7.3

Поверхностная энергия атомного ядра равняется примерно $-17,8A^{1/3}$ МэВ. Радиус атомного ядра $R = 1,3A^{1/3}$ фм. Найти поверхностное натяжение о ядерного вещества. Сравнить найденное значение с поверхностным натяжением ртути ($\sigma_{\text{Hg}} = 470$ эрг/см ^{2}).

7.

3* $\alpha \approx 1,4 \cdot 10^{20}{}_{\text{эрг}}\ /\text{см}^2 \approx 3 \cdot 10^{17}\sigma_{\text{Hg}}$.
Решение. В капельной модели ядра можно по аналогии с жидкой каплей также ввести поверхностное натяжение

$$\sigma = -\frac{E_{\text{пов}}}{S} = -\frac{E_{\text{пов}}}{4\pi R^2} = \frac{17 \cdot 1,6 \cdot 10^{-6} A^{2/3}\ \ni}{4\pi \cdot 1,3^2 \cdot 10^{-26} \cdot A^{2/3}\ \text{см}^2} = 1,4 \cdot 10^{20}\ \ni\ \text{р/см}^2$$

что превышает поверхностное натяжение ртути примерно в $3 \cdot 10^{17}$ раз.

О3.1-7.4

Энергия связи атомных ядер при заданном числе A нуклонов в ядре уменьшается с увеличением числа протонов Z из-за возрастания кулоновской энергии $|\sigma_{\text{к}}| = 0,71\frac{Z^2}{A^{1/3}}$ МэВ. С другой стороны, при отличии числа нейтронов от числа протонов энергия связи уменьшается на величину $\mathscr{E} = \frac{47,4(N-Z)^2}{2A}$ МэВ. Определить при заданном A оптимальное значение Z, при котором энергия связи ядра минимальна. Определить Z/A при $A = 10; 50; 100; 150$ и 200. Найти из справочных данных подходящие изотопы.

7.

4. Решение. Энергия связи ядра
Кроме того,

$$\mathscr{E}_{\text{СВ}} = [Zm_{\text{р}} + (A-Z)m_{\text{n}} - M_{\text{g}}(A,Z)]\,c^2$$

$$\mathscr{E}_{\text{СВ}} = f(A) - \mathscr{E}_{\mathbf{K}} - \mathscr{E}$$

где через $f(A)$ обозначены вклады в энергию связи, не зависящие от Z. Отсюда масса ядра

$$M_{\text{g}}(A,Z) = Zm_{\text{р}} + (A-Z)m_{\text{n}} + [\mathscr{E}_{\mathbf{K}} + \mathscr{E} - f(A)]\,/c^2$$

Приближенно минимум $M_9(A,Z)$ можно найти, считая Z непрерывной переменной и полагая $(\partial M_g/\partial Z)_A = 0$. В результате получим

$$Z = \frac{A}{1,97 + 0,015A^{2/3}}.$$

При пользовании этой формулой нужно брать ближайшее целое значение Z:

A	Z	Ядро	A	Z	Ядро
10	5	${}^{10}_{5}$ B	150	60	${}^{150}_{62}$Sm
50	23	${}^{50}_{20}$ V	200	80	${}^{200}_{80}$Hg
100	44	^{100}Ru			

О3.1-7.5 Устойчивые ядра-изобары при нечетном A

С помощью формулы Вайцзеккера найти заряд Z_0 наиболее устойчивого ядра-изобары при заданном нечетном значении A.
Выяснить, каков характер активности у ядер ^{27}Mg, ^{29}P, ^{37} K, ^{67}Cu.

7.

5. $Z_0 = \frac{A/2}{1+7,5\cdot 10^{-3}A^{2/3}}$. ^{27}Mg – β^--активен; ^{29}P – β^+-активен; ^{37} K - β^+-активен; ^{67}Cu – β^--активен.

В формуле Вайцзеккера находим экстремум, с помощью производной, приравниваем к нулю, получаем уравнение на заряд. Выражаем его, получаем формулу, которая дает ответ.
Округляем.
получаем реакции.
(порешаю потом для других ядер.)

О3.1-7.6*

Разница в энергиях связи ядер трития $^3_1$H и гелия $^3_2$He обусловлена энергией электростатического взаимодействия протонов. Оценить размеры ядра $^3_2$He. Энергии связи ядер $^3_1$H и $^3_2$He равны соответственно $\mathcal{G}_{\text{H}} = 8,482\text{МВ}, \mathscr{O}_{\text{He}} = 7,718\text{МэВ}$.

7.

6. $R_{\text{g}} = \frac{e^2}{\Delta_{\text{cB}}} = 1,9 \cdot 10^{13}$ cm.

Решение. Прежде всего предполагаем, что расстояние между протонами не может быть больше размеров ядра в приближении точечных протонов, т. е. $R_{\text{яд}} \approx \langle r \rangle$. Кроме того, считаем, что разница в энергиях связи обоих ядер $\Delta\mathscr{E}_{\text{СВ}} = \mathscr{E}_{\text{H}} - \mathscr{E}_{\text{He}}$ целиком кулоновского происхождения, т.е. $\Delta\mathscr{E}_{\text{СВ}} = \mathscr{E}_{\text{кул}}$.

Энергия кулоновского взаимодействия протонов в ядре ^{3}He есть

$$\mathscr{E}_{\text{Куа}} = \int \psi^* \frac{e^2}{r} \psi dV$$

Здесь ψ - волновая функция системы нуклонов в ядре, r - расстояние между протонами. Интегрирование идет по объему ядра, т. е. считается, что ядро имеет жесткую форму и вне ядра $\psi \approx 0$. Конкретный вид ψ-функции в данном случае не нужен.

$$\mathscr{E}_{\text{Ку}} = e^2 \int |\psi|^2 \frac{1}{r} dV = e^2 \left\langle \frac{1}{r} \right\rangle .$$

Будем считать, что $\left\langle \frac{1}{r} \right\rangle \simeq \frac{1}{\langle r \rangle}$, и величину $\langle r \rangle$ примем за размер ядра. Таким образом,

$$R_{\text{g}\boldsymbol{A}} = \frac{e^2}{\Delta\varepsilon_{\text{cB}}} = 1,9 \cdot 10^{-13} \text{ cm}.$$

О3.1-7.7

Ядро $^{27}_{14}$Si переходит в «зеркальное» ядро $^{27}_{13}$Al, испытывая β^+ - распад. Максимальная кинетическая энергия вылетевшего позитрона $\sigma_{\max} = 3,48$ МэВ. Оценить по этим данным величину r_0 в формуле для радиуса ядра $R = r_0 A^{1/3}$.

7.

7* $r_0 = 1,4 \cdot 10^{-13}$ cm.

Ре шение. По отношению к ядерным силам протон и нейтрон ведут себя совершенно одинаково. Эта эквивалентность ядерных взаимодействий для протонов и нейтронов проявляется в так называемых зеркальных ядрах, получающихся друг из друга заменой протонов на нейтроны и наоборот. Имен но такими парами и являются ядра $^{27}_{14}\text{Si}\,(14\ \text{р}\ +13\ \text{п})$ и $^{27}_{13}\text{Al}(13\text{р} + 14\ \text{п})$. Одинаковость ядерных взаимодействий для протона и нейтрона носит название зарядовой независимости ядерных сил и является проявлением более общего свойства - изотопической инвариантности сильного взаимодействия.

Если бы изотопическая инвариантность ядерных сил была точным законом природы, то все параметры зеркальных ядер были бы одинаковыми и β раснад был бы запрещен законом сохранения энергии. Кулоновское взаимодействие нарушает зарядовую независимость и делает распад возможным.

$$^{27}_{14}\text{Si} \to {}^{27}_{13}\text{Al} + \text{e}^+ + \upsilon_{\text{e}}.$$

Электрон не может «унести» больше энергии, чем выделяется при распаде. Таким образом,

$$\begin{aligned} m_{\text{e}}c^2 + \mathscr{E}_{\max} &= [M(\text{Si}) - M(\text{Al})]c^2 = \\ &= (m_{\text{p}} - m_{\text{n}})\, c^2 + \frac{3}{5}\frac{e^2}{R}[\, Z_{\text{Si}}\,(Z_{\text{Si}} - 1) - Z_{\text{A1}}\,(Z_{\text{Al}} - 1)] = \\ &= -\,(m_{\text{n}} - m_{\text{p}})\, c^2 + \frac{3}{5}\frac{e^2}{R}(14 \cdot 13 - 13 \cdot 12), \end{aligned}$$

откуда

$$\frac{e^2}{r_0 A^{1/3}} = \frac{5}{78}\left[(m_{\text{n}} - m_{\text{p}} + m_{\text{e}})\, c^2 + \mathscr{E}_{\max}\right].$$

И окончательно, $r_0 = 1,4 \cdot 10^{-13}$ cm.

О3.1-7.8

Найти разность энергий связи для пар зеркальных ядер $\left({}^{11}\text{B},\ {}^{11}\text{c}\right)$ и $\left({}^{13}\text{N}, {}^{13}\text{c}\right)$. Показать, что эта разность в значительной степени обусловлена кулоновским взаимодействием протонов в ядре. Энергию связи ядер взять из таблицы в конце сборника.

7.

8. ${}^{11}\text{C}, {}^{11}\text{B} : \Delta_{\text{СВ}} = 2,8\text{М} \ni \text{В}; \Delta_{\text{К}} \approx 3,19\text{М} \ni \text{В};$
${}^{13}\text{C}, {}^{13}\text{N} : \Delta\mathscr{E}_{\text{СВ}} = 3,0\text{М} \ni \text{В}; \Delta\mathscr{E}_{\text{К}} \approx 3,62\text{М} \supset \text{В}.$
Подсчет $\mathscr{E}_{\text{к}}$ выполняется по формуле $0,71Z^2A^{-1/3}$.

О3.1-7.9

Ядро ${}^{7}_{4}\text{Be}$ «перегружено" протонами и испытывает превращние${}^{7}_{4}\text{Be} \to {}^{7}_{3}\text{Li}$. Массы Этих атомов равны, соответственно, 7,0169 и 1) Радиус ядра определяется по формуле $R_{\text{g}} = r_0A^{1/3}$. При этом коэффициент r_0 при различных аппроксимациях может принимать значения от 1.2 до $1,4 \cdot 10^{-13}$см. В данном задачнике r_0 нринимается равным $1,3 \cdot 10^{-13}$см. 59 7,0160 а. е. м. Определить тип бета-распада, обусловливающего это превращение.

7.

9. K-захват; β^+-распад энергетически невозможен.

О3.1-7.10

В 1942 г. американский физик Аллен измерил максимальную энергию $\mathscr{E}_0$ атомов ${}^{7}\text{Li}$, образующихся в результате K-захвата в ядре ${}^{7}\text{Be}$, и она оказалась равной 50 эВ. Оценить на основе этих данных разность масс атомов ${}^{7}\text{Be}$ и ${}^{7}\text{Li}$.

7.

10. $\Delta Mc^2 \approx \sqrt{2M_{\text{Li}}c^2\mathscr{E}_0} \approx 0,81\text{М В}$.

О3.1-7.11

Определить энергию отдачи ядра атома лития, которое образуется в основном состоянии при поглощении электрона с K-оболочки ядром атома бериллия.

7.

11. $\mathscr{E} \approx 57\ \rho\text{В}$.

О3.1-7.12

Потенциальную энергию взаимодействия нуклонов в дейтроне можно аппроксимировать сферически симметричной прямоугольной ямой (см. задачи 3.16 – 3.18). При этом в системе центра

масс волновая функция основного состояния имеет вне области ямы следующий вид $\psi = Ae^{-xr}/r$, где $A = \text{const}$, $x = 2,3 \cdot 10^{12}\text{см}^{-1}$. Найти красную границу реакции фоторасщепления дейтрона γ-квантами.

7.

12: $\mathscr{E}_{\text{гр}} \approx 2,2\text{М М}$.

Решение. Красная граница фоторасщепления дейтрона определяется энергией связи протона и нейтрона. На рис. 173 изображены потенциальная яма и волновая функция дейтрона. Вне ямы, где $U(r) = 0$, уравнение Шредингера для частицы с приведенной массой $\mu = m_{\text{N}}/2$ имеет вид

$$-\frac{\hbar^2}{2\mu}\Delta_r\psi = \mathscr{E}\psi$$

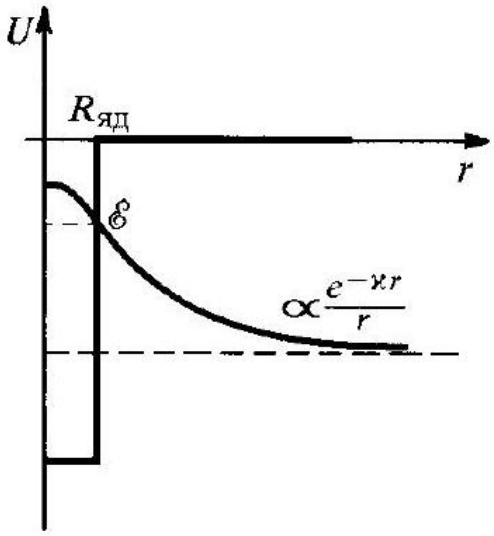


Рис. 173

где $\Delta_r = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}$ - радиальная часть оператора Лапласа.
Подставляя в уравнение $\psi = A\exp(-xr)/r$, получим $x^2\hbar^2 + 2\mu\mathscr{E} = 0$, откуда

$$\mathscr{E} = -\frac{\hbar^2 x^2}{2\mu}.$$

Таким образом, минимальное значение энергии, достаточной для расщепления дейтрона,

$$\mathfrak{E}_{\Gamma p} = \frac{\hbar^2 x^2}{2\mu} = \frac{\hbar^2 x^2}{m_{\mathrm{N}}} \approx 2,23\text{МВВ}$$

О3.1-7.13

* Согласно гидродинамической модели ядра ШтайнведеляЕнсена протоны и нейтроны образуют сжимаемые и свободно проникающие друг в друга жидкости, двигающиеся внутри жесткой оболоч ки исходного ядра. Гигантский резонанс в ядрах соответствует возбуждению противофазных колебаний этих жидкостей, при которых протоны и нейтроны в ядре то пространственно разделяются, то равномерно перемешиваются. Используя формулу Вайцзеккера, оценить рическом ядре с $A = 64(Z = N)$, который возникает при возбуждении волны с $kR = 2,08$, где $k = 2\pi/\lambda$ - волновое число, λ - длина волны, R - радиус ядра. Закон дисперсии этих волн считать линейным ($\omega = ku$, где u - скорость распространения колебаний, равная, как в любой жидкости, $u = \sqrt{K/M}$, где в данном случае K - жесткость ядра относительно смещений нуклонов, M - масса ядра).

7.

13. $\mathscr{E}_{\mathrm{GR}} = \hbar\frac{2,08}{R}\sqrt{\frac{2a_{\mathrm{s}}}{m_{\mathrm{N}}}} \approx 17,7\text{М} \supset \text{В}$, где $a_{\mathrm{s}} = 23,7\text{М В}$ - коэффициент в симметрийном члене в формуле Вайцзеккера, $R = 5,2$ фм.

Решение. Если жесткость системы равна K, то упругая энергия $\mathscr{E} = K\varepsilon^2/2$, где ε - относительное смещение. Возвращающая сила, обусловленная симметрийным членом в формуле Вайцзеккера, стремится восстановить равномерную плотность протонов и нейтронов. Симметрийный член в энергии меняется в расчете на 1 нуклон следующим образом:

$$\mathscr{E}_{\mathrm{s}} = \frac{1}{A}a_{\mathrm{s}}\frac{(A-2Z)^2}{A} = \frac{1}{2}2a_{\mathrm{s}}\left(\frac{N-Z}{A}\right)^2,$$

где $a_{\mathrm{s}} = 23,7\text{М В}$ - коэффициент в формуле Вайцзеккера, N - число нейтронов.

Изменением кулоновской энергии при сжатии протонов вдвое можно пренебречь в силу относительной малости кулоновского члена в формуле Вайцзеккера. Сравнивая $\mathscr{E}_{\mathrm{s}}$ с упругой энергией $\mathscr{E}$ и полагая, что $(N-Z)/A$ - относительное смещение протонов относительно нейтронов, можно сделать вывод, что в расчете на один нуклон жесткость системы $K = 2a_{\mathrm{S}}$. По формуле, данной в условии задачи, скорость распространения колебаний (скорость звука) $u^2 = K/m_{\mathrm{N}} = 2a_{\mathrm{s}}/m_{\mathrm{N}}$, где m_{N} - масса нуклона.

Таким образом, энергия гигантского дипольного резонанса $\mathscr{E}_{\mathrm{GR}}$ в сферическом ядре с $A = 64$ (при $Z = N$)

$$\mathscr{E}_{\mathrm{GR}} = \hbar k u = \hbar \frac{2,08}{R} u = \hbar \frac{2,08}{R} \sqrt{\frac{2a_{\mathrm{s}}}{m_{\mathrm{N}}}} \approx 17,7\mathrm{M} \ni \mathrm{B}$$

Приведем другое решение данной задачи. Подсчитаем изменение энергии, непосредственно возникающее при смещении L нейтронов вправо, а L протонов влево. Тогда в левой половине будет $N/2 - L$ нейтронов и $Z/2 + L$ протонов, а в правой половине ядра $N/2 - L$ нейтронов и $Z/2 + L$ протонов (рис. 174).

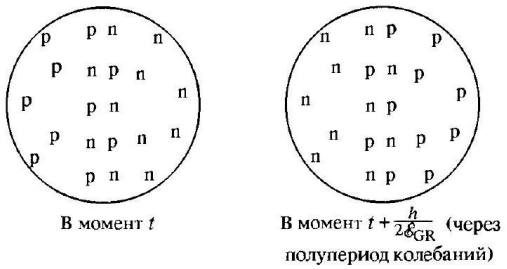


Рис. 174

Полная энергия, связанная с нарушением симметрии, есть

$$\mathscr{E}_{\mathrm{s}} = \frac{(N/2 + L - Z/2 + L)^2}{A/2} a_{\mathrm{s}} + \frac{(N/2 - L - Z/2 - L)^2}{A/2} a_{\mathrm{s}} = \frac{16L^2}{A} a_{\mathrm{S}}$$

Приведем эту формулу к тому же виду $\mathscr{E} = K\varepsilon^2/2$ (см. первое решение). При этом становится очевидно, что максимальное число смещенных протонов или нейтронов равно $A/4$. Таким образом,

откуда $K = 2a_{\mathrm{s}}A$.

$$\mathscr{E}_{\mathrm{S}} = \frac{1}{2} 2a_{\mathrm{s}} A \left(\frac{L}{A/4} \right)^2,$$

Далее легко видеть, что мы приходим к тому же выражению для $\mathscr{E}_{\mathrm{GR}}$, что и в первом решении, поскольку полученное K следует либо привести к одному нуклону, т. е. поделить на A, либо воспользоваться формулой для расчета скорости u, приведенной в условии задачи,

$$u = \sqrt{\frac{K}{M}} = \sqrt{\frac{2a_{\mathrm{s}A}}{Am_N}} = \sqrt{\frac{2a_{\mathrm{s}}}{m_N}}.$$

Заметим, что эта модель достаточно хороно описывает положение гигантского резонанса. Например, в ядре меди, у которого как раз $A = 64$, он наблюдается при энергии возбуждения 16 М МВ.

О3.1-7.14 Три первых ядерных оболочек в оболочечной модели ядра

Согласно оболочечной модели ядра нейтроны и протоны независимо заполняют потенциальную яму. Определить число нуклонов A, которые могут располагаться на трех первых ядерных оболочках, считая потенциальную яму трехмерной параболической.

7.

14. Нейтроны и протоны заполняют свои уровни независимо друг от друга, т. к. они не являются тождественными частицами. Первая оболочка $Z = N = 2; A = 4$ (He). Вторая оболочка $Z = N = 8; A = 16$ (O). Третья оболочка $Z = N = 20; A = 40$ (Ca).

(??? про модель в теории лучше напишу потом.)

О3.1-7.15

*.

Простейшей оболочечной моделью ядра является трехмерный гармонический осциллятор. Считая, что потенциальная яма ядра имеет глубину $U_0 = -70\mathrm{M} \ni \mathrm{B}$, а $U(R_0) = 0$, где R_0 - радиус ядра, оценить энергию связи нуклона для ядра кислорода 168.

7.

15: $\mathscr{E}_{\text{св}} = |U_0| - \frac{5}{2}\hbar\sqrt{-\frac{2U_0}{m_{\text{N}}R_0^2}} \approx 12\text{М}\ni\text{В}$, где m_{N} - масса нуклона.

Решение. Радиус ядра кислорода $^{16}_{8}\text{O}$ $R_0 = 1,3\cdot10^{-13}\sqrt[3]{16} \approx \approx 3,3\cdot10^{-13}$ cm. Потенциальная энергия в однонуклонном приближении описывается выражением

$$U(r) = U_0 + \frac{m\omega^2 r^2}{2}$$

При $r \geqslant R_0$ потенциал $U(r) = 0$, и следовательно

$$\omega = \sqrt{-\frac{2U_0}{mR_0^2}},$$

а уровни энергии имеют вид

$$\mathscr{E}_N = U_0 + \hbar\omega\left(N + \frac{3}{2}\right).$$

Картина уровней изображена на рис. 175. В пренебрежении конечным размером ямы уровни энергии эквидистантны. В силу зарядовой независимости ядерных сил (задача 7.7) уровни протонов и нейтронов в

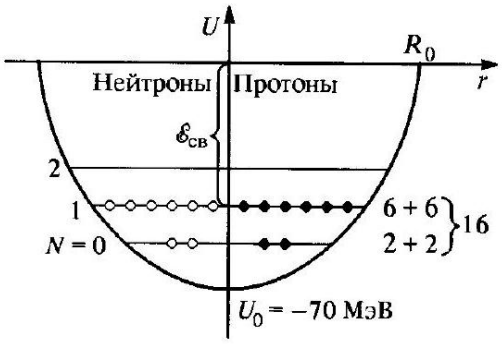


Рис. 175 ядрах с $N = Z$ должны совпадать. В легких ядрах это действительно имеет место, поскольку в них вклад кулоновского взаимодействия в энергию связи незначителен. В случае ядра $^{16}_{8}$ O полностью оказываются заполненными протонные и нейтронные уровни с $N = 0$ и $N = 1$ (дважды магическое число 8 - по протонам и по нейтронам).

На рис. 156 показано также, как отсчитывается искомая энергия связи $\mathscr{E}_{\text{св}}$ (от верхнего заполненного уровня до «потолка» ямы). Таким образом,

$$\mathfrak{E}_{\text{СВ}} \approx |U_0| - \left(N + \frac{3}{2}\right)\hbar\omega$$

где $N = 1$ (внешний нуклон). После преобразований получим

$$\mathscr{E}_{\text{СВ}} = |U_0| - \frac{5\hbar}{2}\sqrt{-\frac{2U_0}{mR_0^2}} \approx 12\text{М}\ni\ \text{В}.$$

О3.1-7.16

Аппроксимируя ядерный потенциал трехмерной параболической ямой глубиной $U_0 = -60$МВ, оценить энергию однонуклонного возбуждения в ядре $^{40}_{20}$ Ca. Считать, что $U(R_0) = 0$, где R_0 - радиус ядра.

7.

16. $\Delta\mathfrak{E} = \hbar\omega = \frac{\hbar}{R_0}\sqrt{-\frac{2U_0}{m}} = 15,8\text{М ЭВ}.$

О3.1-7.17

У ядра дейтерия - дейтрона d - нет стационарных возбужденных состояний, а энергия связи нуклонов составляет $\check{\Xi}_{\text{сВ}} = 2,23$МВ. Аппроксимируя эффективный потенциал нуклоннуклонного взаимодействия трехмерной сферически симметричной прямоугольной потенциальной ямой глубиной $U_0 = -30$М В оценить радиус эффективного потенциала (см. также задачу 3.18).

7.17.

$a^2 = \frac{\pi^2\hbar^2}{8\mu|U_0|}$; $a \approx 1,8 \cdot 10^{-13}$ см, где $\mu = \frac{m_\text{P}}{2}$ - приведенная масса дейтрона. Приведем также результат точного решения, полученного из условия сшивки волновых функций на границе (см. также задачи 3.18 и 3.12):

$$a = \frac{\hbar}{\sqrt{2\mu\left(|U_0| - \mathscr{E}_\text{CB}\right)}} \arccos\frac{\mathscr{E}_\text{CB}}{|U_0|} = 1,82 \cdot 10^{-13} \text{ cm}.$$

7.18.

7.

18. $R_\text{d} = \sqrt{\langle r^2\rangle} = \frac{\hbar}{\sqrt{2m_\text{N}}} \approx 3 \cdot 10^{-13}$ cm, где m_N - масса нуклона. Здесь для оценки можно воспользоваться волновой функцией основного состояния дейтрона (см. задачу 7.12) $\psi \approx Ae^{-xr}/r$, где $\chi = \frac{1}{\hbar}\sqrt{m_\text{N}\mathscr{E}}$.

О3.1-7.19

На рис. 43 изображен спектр низколежащих возбужденных уровней ядра ^{234}U, где $\mathscr{E}$ - энергия уровня, L - квантовое число момента импульса. Показать, что эти уровни сответствуют возбуждению вращения ядра как целого относительно оси, перпендикулярной к оси симметрии ядра. Оценить из этих данных момент инерции J ядра.

7.

19. $J \simeq 1,4 \cdot 10^{-47}\Gamma \cdot \text{ cm}^2$.

О3.1-7.20

Ядро ^{234}U является продуктом распада основного изотопа урана ^{238}U. Определить период полураспада ^{234}U, если его содержание в естественном уране в настоящее время составляет $0,0055\%$. Период полураспада ^{238}U равен $T_8 = 4,51 \cdot 10^9$ лет. Считать, что вначале «наработанного» ^{234}U не было.

7.

20. В силу радиоактивного равновесия между ^{238}U и ^{234}U $\lambda_4 N_4 = \lambda_8 N_8$ (вековое уравнение), откуда

$$\frac{T_4}{T_8} = \frac{\lambda_8}{\lambda_4} = \frac{N_4}{N_8} = 5,5 \cdot 10^{-5}; \quad T_4 = 2,48 \cdot 10^5 \text{ лет}.$$

Период полураспада ^{234}U много меньше возраста Земли ($\approx 10^9$ лет); таким образом, наше предположение о наличии радиоактивного равновесия между ^{238}U и ^{234}U оправдано.

О3.1-7.21

В настоящее время в природном уране содержится $k_8 = 99,28\%^{238}$U и $k_5 = 0,72\%$ ^{235}U. Какое соотношение между ^{238}U и ^{235}U было в момент образования Земли, если возраст Земли равен $4 \cdot 10^9$ лет? Периоды полураспада $T_5 = 0,713 \cdot 10^9$ лет; $T_8 = 4,51 \cdot 10^9$ лет. Вычислить возраст Земли в предположении, что в момент образования Земли содержание ^{235}U и ^{238}U было одинаковым.

О3.1-7.22

Период полураспада ^{234}U равняется $T_4 = 2,48 \cdot 10^5$ лет. Остался ли хотя бы один атом ^{234}U, который существовал в момент образования Земли $-4 \cdot 10^9$ лет тому назад? Как объяснить, что в природном уране содержится примесь ^{234}U в количестве $0,055\%$?

О3.1-7.23

Периоды полураспада ^{238}U и ^{235}U равны соответственно $T_8 = 4,51 \cdot 10^9$ лет и $T_5 = 0,713 \cdot 10^9$ лет. Определить средние времена жизни этих изотопов.

О3.1-7.24

Полагая, что перед α-распадом в ядре образуется самостоятельная α-частица, оценить отношение интенсивностей $_1/_2$ двух групп α-частиц с кинетическими энергиями 6,3 и 5, 7МВ, испускаемых ядрами с $Z = 86$ и $A = 220$. В обоих случаях частоту ударов о «стенку» потенциального барьера считать одинаковой.

О3.1-7.25

Оценить период полураспада $T_{1/2}$ радиоактивного ядра, испускающего α-частицы в энергией 1МВ, если ядро $^{232}_{90}$Th имеет период полураспада $T_{1/2} = 1,4 \cdot 10^{10}$ лет и испускает α-частицы с энергией 4МВ, а для ядра $^{212}_{84}$Po период полураспада равен $T_{1/2} = 3 \cdot 10^{-7}$с и $\mathscr{E}_\alpha = 8,8$МВ.

О3.1-7.26

Энергия α-частиц, испускаемых тяжелыми ядрами ($Z \sim 90$), примерно равна $\mathscr{E}_\alpha \sim 4,5$ МэВ, а период их полураспада $T_\alpha \sim 7 \cdot 10^8$ лет. Оценить период полураспада такого же ядра по отношению к вылету протона той же энергии $\oint_p = 4,5$МВ. Считать задачу одномерной, кулоновский потенциал $U \gg \hat{G}$, а предэкспоненциальный множитель в выражении для проницаемости барьера константой.

О3.1-7.27*

Исследование свойств α-радиоактивных ядер показало, что ядра в области $Z_1 \sim 90$ испускают α-частицы с энергией $\oint_1 \sim 4$ МэВ (например, ядро $^{232}_{90}$Th), а в области редкоземельных элементов, где $Z_2 \sim 65$, - с энергией $\mathscr{E}_2 \sim 2$ МэВ. Оценить период полураспада редкоземельных ядер T_2, если известно, что у тяжелых ядер он лежит в районе $T_1 \sim 10^{10}$, лет. Считать, что α-частицы при распаде преодолевают высокий одномерный потенциальный барьер, т. е. $U \gg \sigma$, а предэкспоненциальный множитель в выражении для проницаемости барьера - константа.

О3.1-7.28

Оценить высоту кулоновского барьера для α-частиц, испускаемых ядрами $^{222}_{86}$r. Какова у этих ядер ширина барьера (туннельное расстояние) для α-частиц с энергией $\mathcal{E} = 5,5$МВ?

О3.1-7.29

При радиоактивном распаде ^{60} Co испускается электрон, спин которого параллелен импульсу. Считая, что электроны вылетают из образца изотропно, оценить, на какой угол повернется диск, подвешенный на нити, если образец кобальта нанесен на одну из поверхностей диска. Толщина диска достаточна для полного поглощения в нем электронов, вылетающих в сторону диска. Активность препарата* $)\frac{dN}{dt} = 0,37$ ТБк $= 0,37 \cdot 10^{12}$ расп/с, модуль кручения нити равен $f = 10^{-6}$ дин см/рад.

О3.1-7.32 Время жизни по регистрируемом времени распада

Удельное содержание изотопа ^{14}C, усвоенного деревом при его жизни, уменьшается затем благодаря β-распаду с $T_{1/2} = 5700$ лет. Какой минимальный возраст дерева можно определить по активности ^{14}C, если регистрируется $N = 10^4$ актов распада? Считать, что скорость образования ^{14}C за счет бомбардировки атмосферы космическими лучами от времени не зависит.

(овч решал, что-то просто в край лень, формулу распада считаем и все... вроде ничего нет сложного.)

О3.1-7.34

Ядро, пролетая через кристалл, подвергается воздействию периодического поля решетки кристалла, в результате чего возможно резонансное возбуждение ядерных уровней (эффект Окорокова смотрите также задачу 4.47). Обусловлен этот эффект тем, что в системе покоя ядра возникает переменное электрическое поле. До какой полной энергии надо разогнать ядро ^{19} F фтора, чтобы при пролете через кристалл вольфрама в нем возбуждался уровень с энергией $\mathscr{E} = 110$ кэВ? Период решетки в направлении движения я,ра $a = 3,2$Å.

О3.1-7.35

Угловой и магнитный момент ядра $^{13}_{6}$C полностью определяется неспаренным нейтроном, находящимся в состоянии $1p_{1/2}$ над полностью заполненной подоболочкой $1p_{3/2}$. Определить магнитный момент μ ядра $^{13}_{6}$C (в ядерных магнетонах Бора). Магнитный момент свободного нейтрона $\mu_{\mathrm{n}} = g_{\mathrm{sn}}\mu_{\mathrm{g}}\ s_{\mathrm{n}} = -1,91\mu_{\mathrm{s}\lambda}$, где $g_{\mathrm{sn}} = -3,82$ - спиновой g-фактор нейтрона, $s_{\mathrm{n}} = 1/2$ - спин нейтрона.

Ук а за н и е. Магнитным моментом ядра принято называть величину максимальной проекции магнитного момента на заданную ось.

О3.1-7.36

Согласно оболочечной модели ядра в ядре $^{15}_{75}$ N неспаренный протон, определяющий его угловой и магнитный моменты, находится в состоянии $1p_{1/2}$ сверх полностью заполненной подоболочки $1p_{3/2}$. Определить величину магнитного момента μ этого ядра (вядерных магнетонах Бора). Магнитный момент свободного протона $\mu_{\mathrm{p}} = g_{\mathrm{sp}}\mu_{\mathrm{gM}}s_{\mathrm{p}} = 2,79\mu_{\mathrm{g}_{\prime}}$, где $g_{\mathrm{sp}} = 5,58$ - спиновой g-фактор протона, $s_{\mathrm{p}} = 1/2$ - спин протона. Смотрите указание к задаче 7.35.

О3.1-7.37*

При учете сверхтонкого взаимодействия интегралом движения является полный угловой момент атома $\mathbf{F} = \mathbf{I} + \mathbf{J}$, где I, J - полные моменты ядра и электронной оболочки соответственно. Энергия сверхтонкого взаимодействия может быть записана в виде $U_{\mathrm{cr}} = A\langle\boldsymbol{\mu}_{\mathrm{e}}\boldsymbol{\mu}_{\mathrm{g}}\rangle$, где $A = \mathrm{const}$, а $\boldsymbol{\mu}_{\mathrm{e}}, \boldsymbol{\mu}_{\mathrm{r}}$ - магнитные моменты электрона и ядра соответственно. Найти отношение сверхтонких расщеплений основного состояния атомов водорода и дейтерия, т. е. расстояний между уровнями с разными значениями F. Спиновые g-факторы протона и нейтрона равны $g_{\mathrm{sp}} = 5,58$ и $g_{\mathrm{sn}} = -3,82$, спины нуклонов в дейтроне параллельны.

7.

37: $\frac{\Delta\varrho^{\mathrm{H}}_{\mathrm{cT}}}{\Delta\varrho^{\mathrm{d}}_{\mathrm{cT}}} = \frac{4}{3}\frac{g_{\mathrm{sp}}}{g_{\mathrm{sp}}+g_{\mathrm{sn}}} = 4,23.$

Решение. В основном состоянии $L = 0$, и магнитный момент имеет чисто спиновую природу. Спин водородного ядра $S_{\mathrm{H}} = 1/2$, а дейтрона $S_{\mathrm{d}} = 1$. Магнитный момент электрона $\mu_{\mathrm{e}} = g_{\mathrm{g}}\mu_{\mathrm{b}}\mathbf{S}_{\mathrm{e}} = 2\mu_{\mathrm{b}}\mathbf{S}_{\mathrm{e}}$, а ядра $\mu_{\mathrm{g}} = g\mu_{\text{яд}}\,\mathbf{S}_{\mathrm{g.}}$. По определению для дейтерия

$$\mu_{\mathrm{g}} = \left(g_{\mathrm{sp}}\mathbf{s}_{\mathrm{p}} + g_{\mathrm{sn}}\mathbf{s}_{\mathrm{n}}\right)\mu_{\text{яд}} = g\mu_{\text{я}}\,\mathbf{s}_{\mathrm{D}}$$

откуда

$$g = \frac{g_{\mathrm{sp}} + g_{\mathrm{sn}}}{2}$$

Для водорода, естественно, $\boldsymbol{\mu_q} = g_{\mathrm{sp}}\,\mu_{\text{яд}}\,\mathbf{S_p}$. Полный момент атома $\mathbf{F} = \mathbf{S}_{\mathrm{e}} + \mathbf{S_g}$, а величина сверхтонкого расщепления

$$\vec{U}_{\mathrm{cr}} = A\cdot 2g\left(\mathbf{S}_{\mathrm{e}}\mathbf{S_g}\right)\mu_{\mathrm{G}}\mu_{\mathrm{gД}} = Ag\left\langle F^2 - S_{\mathrm{e}}^2 - S_{\mathrm{g}}^2\right\rangle\mu_{\mathbf{b}}\mu_{\mathrm{gд}} =$$
$$= Ag\left[F(F+1) - S_{\mathrm{e}}\left(S_{\mathrm{e}}+1\right) - S_{\mathrm{g}}\left(S_{\mathrm{g}}+1\right)\right]\mu_{\mathrm{Б}}\ \mu_{\mathrm{gп}}\ .$$

Для атома водорода $S_{\mathrm{g}} = 1/2, S_{\mathrm{e}} = 1/2$, поэтому возможные значения $F = 1$ или 0 . Для дейтерия, соответственно, $S_{\mathrm{g}} = 1, S_{\mathrm{e}} = 1/2$, а $F = 3/2$ или $1/2$. Поэтому величина сверхтонкого расщепления для водорода

$$\Delta\delta^{\mathrm{H}}_{\mathrm{cr}} = Ag_{\mathrm{sp}}(1\cdot 2 - 0)\mu_{\mathrm{gR}}\mu_{\mathrm{E}} = 2Ag_{\mathrm{sp}}\mu_{\mathrm{gI}}\mu_{\mathbf{\Sigma}},$$

а для дейтерия

$$\Delta\mathscr{E}^{\mathrm{d}}_{\mathrm{CT}} = Ag\left(\frac{3}{2}\cdot\frac{5}{2} - \frac{1}{2}\cdot\frac{3}{2}\right)\mu_{\mathrm{gI}}\mu_{\mathrm{E}} = 3Ag\mu_{g\Omega}\mu_{\mathrm{b}}$$

Таким образом, $\frac{\Delta\mathscr{C}^{\mathrm{H}}_{\mathrm{cr}}}{\Delta\mathcal{E}^{\mathrm{d}}_{\mathrm{cr}}} = \frac{2g_{\mathrm{sp}}}{3g} = \frac{4}{3}\frac{g_{\mathrm{sp}}}{g_{\mathrm{sp}}+g_{\mathrm{sn}}} = 4,23.$

7. Ядерные модели. Радиоактивность. Эффект Мессбауэра SOLUTIONS

7.

21. $k_8(t) = \frac{k_8}{1+k_5\left[e^{(\lambda_5-\lambda_8)t}-1\right]\cdot 10^{-2}}, \quad k_5(t) = 100 - k_8(t).$

Если подставить числовые значения, то получается, что $4 \cdot 10^9$ лет тому назад содержание ^{235}U составляло $16,08\%$. Примерно $6 \cdot 10^9$ лет тому назад содержания ^{235}U и ^{238}U могли быть равными. Конечно, в момент образования Земли в ее составе имелись и другие изотопы урана (см. задачу 7. 22).

7.

22. С момента образования Земли за время $t = 4 \cdot 10^9$ лет содержание ^{234} U на Земле должно уменьниться в $e^{(t\ln 2)/\tau_4} \approx e^{11180} \approx 10^{4855}$ раз. Если даже предположить, что в момент образования Земли на ней существовали только изотопы ^{234}U, то и тогда на Земле уже давно не осталось бы ни одного атома ^{234}U. Изотоп ^{234}U существует в природе благодаря α-распаду ^{238}U и β^--распадам ^{234}Th и ^{234} Pa

$$^{238}_{92}\mathrm{U} \underset{4{,}5\cdot 10^9 \text{ лет}}{\alpha} {}^{234}_{90}\mathrm{Th} \xrightarrow[24 \text{ дня}]{\beta^-} {}^{234}_{91}\mathrm{Pa} \underset{6{,}7 \text{ час}}{\beta^-_{92}} {}^{234}_{9}\mathrm{U}.$$

Содержание ^{234}U находится из условия радиоактивного равновесия (см. задачу 7.20).

7.

23. $\frac{T_8}{\ln 2} = 6,45 \cdot 10^9$ лет; $\frac{T_5}{\ln 2} = 1,016 \cdot 10^9$ лет.

7.

24. В связи с тем, что проницаемость кулоновского барьера экспоненциально зависит от ширины барьера, то ответ задачи оказывается чрезвьн чайно чувствителен к выбору приближения. Приведем три возможных формы ответа:

1. $\frac{1}{2} = \exp\left\{-\frac{4(Z-2)e^2\sqrt{2m_a}}{\hbar}\left[\frac{1}{\sqrt{\mathscr{E}_1}}\arccos\sqrt{\frac{\mathscr{E}_1}{U_0}} - \right.\right.$

$$\left.\left. -\frac{1}{\sqrt{\epsilon_2}}\arccos\sqrt{\frac{\varrho_2}{U_0}} + \sqrt{\frac{\mathscr{E}_2}{U_0}\left(1-\frac{\mathscr{C}_2}{U_0}\right)} - \sqrt{\frac{\mathscr{E}_1}{U_0}\left(1-\frac{\mathscr{E}_1}{U_0}\right)}\right]\right\} = 744$$

2. $\frac{\mathscr{I}_1}{2} = \exp\left[\frac{2\pi(Z-2)e^2\sqrt{2m_a}}{\hbar}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{1}}\right)\right] = 942;$

3. $\frac{\mathscr{I}_1}{\mathscr{I}_2} = \exp\left[\frac{8(Z-2)e^2}{\hbar}\sqrt{2m_\alpha}\left(\frac{1}{\sqrt{\mathscr{E}_2}} - \frac{1}{\sqrt{1}}\right)\right] = 6130,$

где $U_0 = \frac{2(Z-2)e^2}{R}$, R - радиус ядра с массовым числом $A-4$.
Формулы 1)-3) получены для случая, когда вне ядра α-частица описывается плоской волной (обрыв барьера при $r = R$), что приближенно справедливо, если энергия α-частицы мала по сравнению с высотой кулоновского барьера. Полученные формулы справедливы также при вылете α-частицы «из центра» ядра, когда можно не учитывать центробежный барьер. При этом формула 1) представляет собой результат точного интегрирования; формула 2) является предельным случаем при $U_0 \to \infty$, а формула 3) есть результат интегрирования при $U(r) \gg$.

7.

25. Зависимость периода полураспада от энергии (в МэВ) хорошо описывается законом Гейгера - Неттола

$$\lg T_{1/2} \approx A + \frac{B}{\sqrt{\varepsilon_a}}$$

Из условий задачи константы $A \approx -56,5; B \approx 148,3$. Искомый период полураспада равен $T_{1/2} \simeq 3{\cdot}10^{84}$ лет.

7.

26.

$$\frac{T_{\text{p}}}{T_a}=\frac{\lambda_a}{\lambda_{\text{p}}}=\exp\left[\frac{4\sqrt{2}Ze^2}{\hbar\sqrt{\epsilon}}\left(Z_\alpha\sqrt{m_\alpha}-Z_\rho\sqrt{m_{\text{p}}}\right)\right]=e^{-169},T_{\text{p}}\approx 9\cdot 10^{-57}\text{с}.$$

В силу столь малых времен естественная протонная радиоактивность не наблюдается. Она обнаруживается экспериментально лишь в том случае, когда ей предшествует более медленный β-распад.

7.

27: $T_2\sim 10^{12}$ лет.
Решение. При выполнении условия $U\gg\mathscr{E}$ и $Z\gg 2$ проницаемость барьера равна (см. задачу 3.36)

$$D\approx\exp\left(-\frac{4\sqrt{2m}Z_uZe^2}{\hbar\sqrt{\varepsilon}}\right),$$

тогда $\frac{T_1}{T_2}=\exp\left[\frac{4\sqrt{2m}Z_\alpha e^2}{\hbar}\left(\frac{Z_1}{\sqrt{\zeta_1}}-\frac{Z_2}{\sqrt{\zeta_2}}\right)\right]\approx e^{-4,9}=7\cdot 10^{-3}$ (здесь $Z_\alpha=2$). Откуда $T_2\sim 10^{12}$ лет.
Заметим, что реальное ядро $^{152}_{65}$Tb имеет период полураспада $1,1\cdot 10^{14}$ лет при энергии α-частицы 2, 14М ЭВ.

7.

28. $U_0=\frac{2(Z-2)e^2}{R}=30,7\text{МВ};\quad d=\frac{2(Z-2)e^2}{\mathscr{E}}-R=36$ фм, где $R=r_0A^{1/3}\approx 7,9$ фм - радиус ядра.

7.

29: $\varphi=\frac{\dot{N}\hbar}{8f}\approx 5\cdot 10^{-11}$ рад $=50$ прад.
Решение. Электроны, вылетающие с поверхности диска, делятся на две равные части. Одна из них поглощается диском, а вторая, вылетающая в телесный угол 2π, покидает диск, унося момент

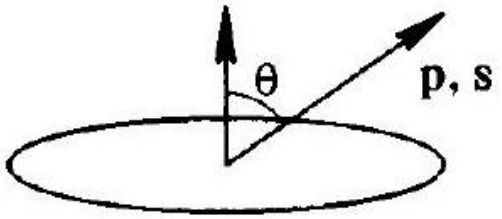


Рис. 176 импульса. Электрон, вылетающий с поверхности диска под углом θ (рис. 176), уносит момент импульса $\hbar/2$. Проекция этого момента на ось вращения равна $(\hbar/2)\cos\theta$. Поскольку все направления вылета равновероятны, то изменение момента импульса в единицу времени $\frac{dL}{dt}=\frac{\dot{N}}{2}\frac{\hbar}{2}\overline{\cos\theta}$, где черта означает усреднение по телесному углу 2π.

$$\overline{\cos\theta}=\frac{1}{2\pi}\int_\Omega\cos\theta d\Omega=\frac{1}{2\pi}\int_0^{\pi/2}2\pi\sin\theta\cos\theta d\theta=\frac{1}{2}$$

Таким образом $dL/dt=\dot{N}\hbar/8$. С другой стороны

$$\frac{dL}{dt}=f\varphi$$

откуда и следует ответ

$$\varphi=\frac{\dot{N}\hbar}{8f}\approx 5\cdot 10^{-11}\text{ рад}.$$

7.

30. $t = 1,57 \cdot 10^{17}$с $\approx 5 \cdot 10^9$ лет (практически равно времени жизни Вселенной). Т. е. таких условий на Земле, по-видимому, не существовало.

7.

31: $\tau_{\text{дип}} \simeq 2 \cdot 10^{-16}$с; $\tau_{\text{квад}} \simeq 5 \cdot 10^{-13}$с.
Решение. Число γ-квантов, излучаемых в единицу времени,

$$\frac{W}{\hbar\omega} = \frac{1}{\tau}$$

где τ - время жизни возбужденного уровня относительно излучения.
Дипольный момент $d = eR\sin\omega t$, где R - радиус ядра. Поэтому $\ddot{d} \approx eR\omega^2$ с точностью до коэффициента порядка единицы. Классическое выражение (данное в условии) для энергии дипольного излучения в единицу времени можно привести к виду:

$$W \approx \frac{2}{3c^3} e^2 R^2 \omega^4.$$

Таким образом, для дипольного излучения время жизни возбужденного уровия

$$\tau_{\text{дип}} = \frac{\hbar\omega}{W} \simeq \frac{3\hbar c^3}{2e^2 R^2 \omega^3}.$$

Если ввести $\neq \frac{c}{\omega} \simeq \frac{200}{\mathscr{E}[\text{ МэВ }]}[]$ - приведенную длину волны γ-кванта с энергией $\mathscr{E}$ в МэВ, то искомое время жизни

$$\tau_{\text{дип}} \simeq \frac{\hbar c}{e^2\omega}\left(\frac{\lambda}{R}\right)^2 \simeq \frac{8 \cdot 10^{-20}}{\mathscr{E}}\left(\frac{200}{\mathscr{E}R}\right)^2 [\text{с}].$$

При $\mathscr{E} = 1$ МэВ и $R = 4$ фм (условие задачи) формула дает Т $= 2 \cdot 10^{-16}$с.
Для мультипольных (в частности - квадрупольных) переходов оценочная формула будет примерно такой же. Изменится только степень размера ядра (размера системы). Из электродинамики известно, что при разложении электрического поля в ряд по мультиполям параметром разложения является отношение размеров системы к расстоянию до точки наблюдения (безразмерная величина). Если в дипольный момент входит R в первой степени, т. е. $d \sim eR$, то в квадрупольный момент входит R^2, а в момент порядка m - R^m. Таким образом, время излучения с моментом m равняется

$$\tau_m \approx \frac{8 \cdot 10^{-20}}{\mathscr{E}}\left(\frac{200}{\mathscr{E}R}\right)^{2m}$$

Так, для $m = 2$ (квадруполь) $R = 4$ фм, $\mathscr{E} = 1$М ВВ, $\text{Т}_{\text{квад}} \approx 5 \cdot 10^{-13}$с.

7.

32. $t = -\frac{T_{1/2}\ln 0,1}{\ln 2} \approx 1,9 \cdot 10^4$ лет.

7.

33. $t_{\min} = \frac{0,01T_{1/2}}{\ln 2} \approx 80$ лет.
Указание. Минимальный возраст, который можно определить, ограничивается статистикой отсчетов.

7.

34. $\beta^2 = \left(\frac{v}{c}\right)^2 = \frac{[\Delta\mathscr{E}a/(ch)]^2}{1+[\Delta\mathscr{E}a/(ch)]^2}$, где $\Delta\mathscr{E} = 110$ кэВ; $\gamma = \left(1-\beta^2\right)^{-1/2} = \frac{\Delta\mathscr{E}a}{ch} \approx 28,5; \mathscr{E} = \gamma M_0 c^2 \approx 510$ ГэВ.
Указание. Для возбуждения уровня в системе покоя ядра нужна ча стота, определяемая из условия $h\nu = \Delta$. Частота возбуждения есть $\nu' = \frac{v}{a'} = \frac{v}{a\sqrt{1-v^2/c^2}}$, поскольку эффективный размер решетки сокращается в направлении движения ядра.

7.

35: $\mu = -1,9\,(-\mu_{\text{яд}}\,/3) \approx 0,64\mu_{\text{gд}}$.

Решение. Векторная модель сложения угловых моментов ядра ($\mathbf{J} = \mathbf{L} + \mathbf{S}$) и магнитных моментов ($\mu_{\text{сум}} = \mu_{\mathbf{L}} + \mu_{\mathbf{S}}$) в самом общем виде изображена на рис. 177, на котором векторы моментов импульса должны быть отложены в единицах $\hbar$, а векторы магнитных моментов - в ядерных магнетонах Бора. Но в силу того, что для протона $g_{l\text{p}} = 1$, для нейтрона
$g_{l\text{n}} = 0$ (в силу его электрической нейтральности), а спиновые g-факторы, соответственно, $g_{sp} = 5,58$ и $g_{sn} = -3,82$, рис. 177 не отражает (в смысле масштабов) условие задачи, а лишь помогает по-

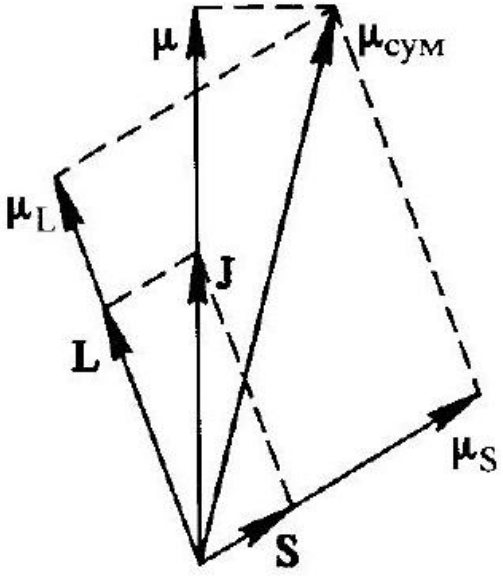


Рис. 177 нять правило сложения моментов. Средний магнитный момент ядра может быть направлен только вдоль J, единственного сохраняющегося вектора в системе, $\langle \mu_{\text{сум}} \rangle = \mu = g_{\mathbf{J}}\mu_{\text{яд}}\,\mathbf{J}$. Умножим это равенство скалярно на и усредним по состоянию с заданными J, L, S. Тогда в силу того, что J - сохраняющийся вектор, его можно внести под знак усреднения, и мы получаем:

$$\langle \mu_{cy}\mathbf{J} \rangle = g_{\mathbf{J}}\mu_{\boldsymbol{g}} \left\langle \mathbf{J}^2 \right\rangle$$

Поскольку $\mu_{\text{L}} = g_{\text{L}}\mu_{\text{яд}}\,\mathbf{L}$ и $\mu_{\text{S}} = g_{\text{S}}\mu_{\text{яд}}\,\mathbf{S}$, то

$$g_{\mathbf{S}}\langle \mathbf{SJ} \rangle + g_{\mathbf{L}}\langle \mathbf{LJ} \rangle = g_{\mathbf{J}} \left\langle \mathbf{J}^2 \right\rangle$$

Используя теорему косинусов, получим

$$\frac{g_{\text{S}} \left\langle \mathbf{J}^2 + \mathbf{S}^2 - \mathbf{L}^2 \right\rangle}{2} + \frac{g_{\text{L}} \left\langle \mathbf{J}^2 + \mathbf{L}^2 - \mathbf{S}^2 \right\rangle}{2} = g_{\text{J}} \left\langle \mathbf{J}^2 \right\rangle$$

В квантовой физике справедливы соотнонения

$$\left\langle \mathbf{J}^2 \right\rangle = J(J+1); \left\langle \mathbf{S}^2 \right\rangle = S(S+1); \left\langle \mathbf{L}^2 \right\rangle = L(L+1)$$

Используя их, получим

$$g_{\mathbf{J}} = \frac{g_{\mathbf{S}} + g_{\mathbf{L}}}{2} + \frac{g_{\mathbf{S}} - g_{\mathbf{L}}}{2} \cdot \frac{S(S+1) - L(L+1)}{J(J+1)}$$

В нашем случае магнитный момент ядра определяется состоянием нейтрона, находящегося на уровне $1p_{1/2}$, т.е. для нейтрона $g_{\mathbf{L}} = g_{l\text{n}} = 0$, $g_{\mathbf{S}} = g_{\text{sn}} = -3,82, S = 1/2; L = 1; J = 1/2$. Подставляя эти данные, получим $g_{\mathbf{J}} = 1,91 \cdot \frac{2}{3} \approx 1,273; \mu = g_{\mathbf{J}}\mu_{\text{я}}\,J \approx 0,64\mu_{\text{яд}}$.

7.

36. $\mu \approx -0,26\mu_{\text{яд}}$.

18.2.3 Problems about radioactivity 2

O3.1-7.38

Спин ядра атома лития (его полный угловой момент) $I = 3/2$. При учете сверхтонкого взаимодействия интегралом движения является полный момент атома $\mathbf{F} = \mathbf{I} + \mathbf{J}$($\mathbf{J}$ - угловой момент электронной оболочки). Найти два возможных значения магнитного момента атома лития, находящегося в состоянии $2^2P_{1/2}$. Собственным магнитным моментом ядра пренебречь.

O3.1-7.39

Свободное покоящееся атомное ядро массой M переходит из возбужденного состояния в основное, испуская γ-квант. Найти энергию γ-кванта и энергию отдачи R, если энергия возбуждения равнялась $\mathscr{E}$. Получить числовой ответ для $^{191}_{77}$Ir если $\mathscr{E} = 129$ кэВ.

O3.1-7.40

Свободное покоящееся атомное ядро массой M переходит в возбужденное состояние с энергией возбуждения $\mathscr{E}$, поглощая γ-квант. Определить энергию γ-кванта и энергию отдачи ядра R.

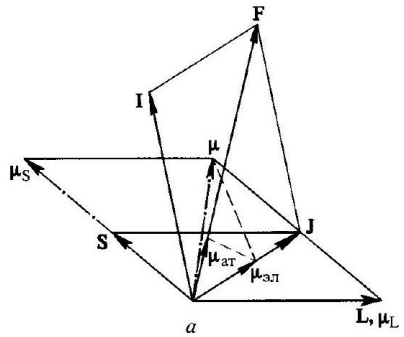
Многие другие еще не выгружены

(другие не выгружал пока что, итак есть над чем подумать.)

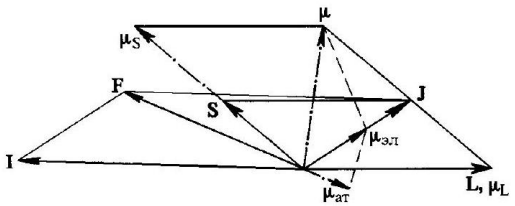
7. Ядерные модели. Радиоактивность. Эффект Мессбауэра SOLUTIONS

7.

38*: $\langle \mu_{\text{ar}} \rangle (F = 1) = -\frac{\mu_{\text{E}}}{6}; \langle \mu_{\text{at}}(F = 2) \rangle = \frac{\mu_{\text{E}}}{3}$.



a



σ

Рис. 178

Решен ие. Магнитный момент атома $\mu_{\text{ат}}$ складывается из магнитных моментов электронной оболочки и ядра $\mu_{\text{ат}} = \mu_{\text{e}} + \mu_{\text{g}} \simeq \mu_{\text{e}}$, т. к. $|\mu_{\text{e}}| \gg |\mu_{\text{g}}|$. В состоянии с заданным J средний магнитный момент электрона

$$\bar{\mu}_{\text{e}} = g_{\mathbf{j}} \mu_{\text{E}} \mathbf{J}, \quad \text{где} \quad g_{\mathbf{J}} = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}.$$

В нашем случае $g_{\mathbf{J}} = 2/3$. При наличии взаимодействия ядра с электронами сохраняющимся вектором является $\mathbf{F} = \mathbf{J}+\mathbf{I}$, и средний магнитный момент атома $\langle \overline{\boldsymbol{\mu}}_{\text{a}} \rangle$ должен быть направлен по $\mathbf{F}$, т. е. $\langle \boldsymbol{\mu}_{\text{at}} \rangle = \mu \mathbf{F}$. Умножая обе части скалярно на $\mathbf{F}$ и внося вектор $\mathbf{F}$ под знак усреднения, получим $\mu \langle \mathbf{FF} \rangle = g_J \langle \mathbf{JF} \rangle \mu_{\mathbf{6}}$, или

$$\mu \left\langle \mathbf{F}^2 \right\rangle = \mu_{\mathbf{E}} g_J \frac{1}{2} \left\langle \mathbf{F}^2 + \mathbf{J}^2 - \mathbf{I}^2 \right\rangle. \quad \text{Отсюда} \quad \mu = g_J g_F \mu_{\mathbf{E}}$$

где $g_F = \frac{1}{2} + \frac{J(J+1)-I(I+1)}{2F(F+1)}$.
Поскольку $I = 3/2, J = 1/2$, то или $F = 2$ и $g_F = +1/4$ или $F = 1$ и $g_F = -1/4$. Следовательно,

$$\langle \mu_{\text{aT}}(F=2) \rangle = \frac{2}{3}\left(\frac{1}{4}\right)\mu_{\text{G}} \cdot 2 = \frac{\mu_{\text{E}}}{3}.$$

$$\langle \mu_{\text{aT}}(F=1) \rangle = \frac{2}{3}\left(-\frac{1}{4}\right)\mu_{\text{E}} \cdot 1 = -\frac{\mu_{\text{E}}}{6};$$

Примечание. Возможность такого подхода для вычисления $\mu_{\text{ат}}$ связана с малостью энергии сверхтонкого взаимодействия по сравнению с энергией спин-орбитального взаимодействия. Строго говоря, в векторной модели атома нужно сложить μ_S и μ_L и спроецировать сумму на направление **F**. Мы же проецируем сначала на **J**, а потом на **F**. Частота прецессии **J** вокруг F много меньше частоты прецессии L и S вокруг J (см. рис. 178*а* и б).

7.

39*. Решение. При испускании γ-кванта должны выполняться законы сохранения энергии и импульса

$$\mathscr{E} = \hbar\omega + R$$

$$\frac{\hbar\omega}{c} = p_R = \frac{1}{c}\sqrt{R\left(2Mc^2 + R\right)}$$

где p_R - импульс ядра после испускания γ-кванта. Решая эти уравнения, получим

$$R = \frac{\mathfrak{E}^2}{2\left(Mc^2 + \mathscr{E}\right)} \approx \frac{\mathfrak{E}^2}{2Mc^2} = 0,0468 \text{ эВ}$$

$$\hbar\omega = \mathscr{E} - \frac{\mathscr{E}^2}{2Mc^2} \approx \mathscr{E} = 129\text{k}$$

7.

40. $R \approx \frac{\mathscr{E}^2}{2Mc^2}; \hbar\omega = \mathscr{E} + R.$

7.

41. Изменение энергии γ-кванта из-за эффекта Доплера $\Delta\mathscr{E} = \mathscr{E}\frac{v}{c}$. Полагая $\Delta\mathscr{E} = \Gamma/6$, получаем $v/c = 6 \cdot 10^{-12}, v = 0,18$ см/с.

7.

42. Условие резонансного поглощения принимает вид $T_{\text{эфф}} \geq \frac{R}{4k_{\text{L}}}$. Поскольку $R = \frac{\mathscr{G}_\gamma^2}{2Mc^2} = \frac{\mathscr{C}_\gamma^2 N_{\text{A}}}{2Ac^2}$, то $T \gtrsim \frac{\mathfrak{G}_\gamma^2 N_{\text{A}}}{8k_{\text{D}}Ac^2} \approx 135$ K.

7.

43. При излучении γ-кванта энергия отдачи R воспринимается всем кристаллом и поэтому $\Delta\mathscr{E} = R = \frac{\varrho_\gamma^2}{2Mc^2} = 1,5 \cdot 10^{-25\text{эВ}}$.

7.

44. Смещение частот $\frac{\Delta\omega}{\omega} = \frac{R^2\Omega^2}{2c^2}$. Если $\frac{\Delta\omega}{\omega} = \frac{1}{3} \cdot 10^{-13}$, то $\Omega = 74$ рад/с.

7.

45. $v = \frac{\mathscr{E}}{2mc} \approx 10^4$ cm/c.

7.

46. $h = \frac{\Gamma c^2}{100 \S_\gamma g} \approx 28$ м, где g - ускорение свободного падения.

7.

47* Решение. Из-за различия эффективных температур излучателя и поглотителя частоты излученного и поглощенного γ-квантов будут смещены на величину порядка $\delta v \simeq v\frac{k_\text{B}\delta T_\text{эфф}}{Mc^2} = v\frac{R\delta T_\text{эфф}}{Ac^2}$, где R - универсальная газовая постоянная, A - атомная масса железа. Именно это смещение должно быть меньше гравитационного $\Delta v = v\frac{gh}{c^2}$ (см. задачу 1.4). Разность температур эквивалентна высоте $\delta h = \frac{R\delta T_\text{эфф}}{Ag} \simeq 15$ м, что сравнимо с высотой башни в эксперименте Паунда и Ребки. Таким образом, для того, чтобы при помощи эффекта Мессбауэра можно было наблюдать гравитационное смещение частоты γ-квантов, температуры излучателя и поглотителя должны быть одинаковыми с очень высокой степенью точности.

7.

48. $H = \frac{10hc^2}{g\tau\varrho} \approx 400$ m.

7.

49. $m = \frac{^2\tau}{\hbar c^2} \approx 5,3 \cdot 10^{-13}\Gamma; b = \left(\frac{3m}{4\pi\rho}\right)^{1/3} \approx 0,25$ мКМ.

7.

50. $\mathscr{E}_\nu = \frac{\Delta\mathscr{E}^m c^2}{2\mathscr{E}_\gamma} \approx 960\kappa$.

Решение. Естественная ширина возбужденного состояния очень мала и равна $\delta\varnothing = \hbar/\tau = 1,5 \cdot 10^{-2}$ эВ. Уширение возникает из-за доплеровского сдвига, связанного с отдачей ядра при испускании нейтрино. Согласно закону сохранения импульса $p_\text{яд} = \mathscr{E}_\gamma/c$, а доплеровский сдвиг равен

$$\Delta(h\nu) = h\nu\frac{v}{c} = \frac{\mathscr{E}_\gamma\mathscr{E}_v}{mc^2} = \frac{\Delta\mathscr{E}}{2}$$

откуда следует

$$\mathscr{E}_v = \frac{\Delta\mathscr{E}^m c^2}{2\mathscr{E}_\gamma} \approx 960 \text{ кэВ}.$$

7.

51. $\tau \approx \frac{\hbar}{(\Delta - 2\delta_\text{доп})} \approx 10^{-17}$с, где $\delta_\text{доп} \approx 160$ В.

Указание. При испускании γ-кванта с энергией 5 МэВ ядро испытывает отдачу, и поэтому линия излучения с энергией $1,5$М МВ оказывается уширенной на $2\delta\mathscr{E}_\text{доп}$.

7.

52. При переходах излучаются магнитно-дипольные (M1) γ-кванты с моментом и четностью 1^+(см. также задачу 7.57). Рассматривая крайние
компоненты расщепления ($\Delta v = 10,5\text{m/c}$), соответствующие изменению спина ядра ($-3/2 \to -1/2$ и $+3/2 \to +1/2$), получим

$$B = \frac{\mathscr{E}_0 \Delta v}{c\mu_{\text{яд}}\left(g_{1/2} + 3g_{3/2}\right)} \simeq 330\kappa\text{Гс}$$

7.

53: $\mathscr{E}_0 = -8,4\text{M эВ}$.
Решение. Предположим, что ядро - равномерно заряженный шар радиусом R (см. задачу 4.41 и рис. 135 к ней). Мюон является лептоном, поэтому он может взаимодействовать с ядром только за счет электромагнитных сил. Тогда потенциальная энергия мюона внутри ядра

$$U(r < R) = -\frac{3}{2}\frac{Ze^2}{R}\left(1 - \frac{r^2}{3R^2}\right) = -U_0 + \frac{Ze^2}{2R^3}r^2, \text{ где } U_0 = \frac{3Ze^2}{2R}$$

Видно, что это потенциал трехмерного изотропного гармонического осциллятора

$$U(r) = -U_0 + \frac{m_\mu \omega^2 r^2}{2}$$

где $\frac{m_\mu \omega^2}{2} = \frac{Ze^2}{2R}$, откуда следует, что $\omega^2 = \frac{Ze^2}{m_\mu R^3}$.
Подсчет дает $U_0 = \frac{3Ze^2}{2R} \approx 23\text{M}$; ; энергия основного состояния $\mathscr{E}_0 = -U_0 + \frac{3}{2}\hbar\omega; \hbar\omega = \sqrt{\frac{\hbar^2 Ze^2}{m_\mu R^3}} = 9,73$ МэВ. Окончательно, $\mathscr{E}_0 = -8,4\text{M МВ}$

7.

54. Для оценки областй локализации можно принять, что она совпадает с амплитудой колебаний трехмерного гармонического осциллятора в основном состоянии

$$\sqrt{\overline{r^2}} = \sqrt{\frac{3\hbar}{m_\mu}\sqrt{\frac{m_\mu R^3}{Ze^2}}} = 1,06 \cdot 10^{-12} \text{ cm}$$

и больше радиуса ядра свинца $R_{\text{Pb}} = 7,7 \cdot 10^{-13}$ cm.

7.

55. $M = 5N(t)m_\alpha \approx 3,2 \cdot 10^{-6}$ г, где число расщепившихся ядер $N(t) \approx \approx N_0 \frac{t \ln 2}{T_{1/2}} = 0,975 \cdot 10^{17}$.

7.

56. $M \approx 300$ т (точно по Маяковскому).

7.

57: $I_{\text{кон}} = \frac{1}{2}$; $2s_{1/2}$-состояние.
Решение. Уравнение Шредингера для осциллятора допускает разделение переменных как в прямоугольной, так и в сферической системе координат. С этим же связано и случайное вырождение уровней энергии в данном потенциале. В декартовой системе уровни осциллятора характеризуются квантовым числом $N = n_x + n_y + n_z$. В сферической системе можно характеризовать их по моменту l и радиальному квантовому числу n_r. При этом $N = 2n_r + l$, а уровни записываются как $(n_r + 1)\,l$. Таким образом, $N = 0$ соответствует $n_r = l = 0$, т. е. это $1s$-состояние. $N = 1$ соответствует $n_r = 0$, $l = 1$, и это $1p$-состояние. $N = 2$ соответствует $n_r = 1, l = 0$ и $n_r = 0, l = 2$,

т. е. это $2s$ и $1d$-состояния, которые в данном приближении вырождены. Учет спин-орбитального взаимодействия приводит к расщеплению $1p$-состояния на $1p_{3/2}$ и $1p_{1/2}$; $1d$-состояния на $1d_{5/2}$ и $1d_{3/2}$. Как показывает эксперимент, в ядре уровень с болыним j лежит ниже по энергии.

При поглощении фотона $E1$ ($j = 1$ - момент импульса фотона) должны выполняться правила отбора

$$|I_{\text{кон}} - I_{\text{нач}}| \leqslant j \leqslant I_{\text{кон}} + I_{\text{нач}}$$

где $I_{\text{кон}}$ и $I_{\text{нач}}$ - конечное и начальное значения спина ядра. Ядро $^{13}_{6}$ С имеет $2 \cdot 2 = 4$ нуклона на оболочке с $N = 0$ и $2 \cdot 6 = 12$ нуклонов на оболочке с $N = 1$. Остается один нейтрон из незаполненной подоболочки в состоянии $1p_{1/2}$ (см. указание к задаче). Для одного нуклона с моментом l четность состояния равна $P = (-1)^l$ ($l = 1$ для состояния $1p_{1/2}$). Таким образом,

$$\left| I_{\text{КОН}} - \frac{1}{2} \right| \leqslant 1 \leqslant I_{\text{КОН}} + \frac{1}{2}$$

Кроме того, должен выполняться закон сохранения четности состояний

$$P_{\text{кон}} \cdot P_{\text{На}} = \begin{cases} (-1)^J & \text{для } EJ - \text{ фотонов;} \\ (-1)^{J+1} & \text{для } MJ - \text{ фотонов ,} \end{cases}$$

где $P_{\text{кон}}$ и $P_{\text{нач}}$ - четности конечного и начального состояний ядра, откуда следует, что конечная четность должна быть равна $P_{\text{кон}} = +1$. С другой стороны, $p_{\text{кон}} = (-1)^{l_{\text{кон}},}$ где $l_{\text{кон}}$ - орбитальный момент конечного состояния. Таким образом, получается, что оно четное. А значит, подходят два нуклонных состояния из $N = 2$: состояние $2s_{1/2}$ ($l_{\text{кон}} = 0$)

$$\left| \frac{1}{2} - \frac{1}{2} \right| \leqslant 1 \leqslant \frac{1}{2} + \frac{1}{2}, \quad \text{т. е.} \quad (0 \leqslant 1 \leqslant 1)$$

а также состояние $1d_{3/2}$ ($l_{\text{кон}} = 2$)

$$\left| \frac{3}{2} - \frac{1}{2} \right| \leqslant 1 \leqslant \frac{3}{2} + \frac{1}{2}, \quad \text{т. е.} \quad (1 \leqslant 1 \leqslant 2)$$

Условию задачи удовлетворяет состояние с наименьшей энергией $2s_{1/2}$, спин ядра $I_{\text{кон}} = \frac{1}{2}$.

7.

58. $I_{\text{кон}} = \frac{3}{2}$; $1d_{3/2}$-состояние.

7.

59. $k = \frac{M_{\text{Т}}}{M_{\text{П}\pi}} = \left(\frac{\cdot\sqrt{2m_\alpha (??)_\alpha} N_{\text{А}} \ln 2}{4 g T_{1/2} A} - 1 \right)^{-1} \approx 0,52.$

7.

60. $\mu_{\text{d}}^{(1)} = \frac{\mu_{\text{яд}}}{2} \left[\frac{3}{2} - \frac{5,58-3,82}{2} \right] = 0,31 \mu_{\text{яд}}$ - для случая ls-связи;
$\mu_{\text{d}}^{(2)} = \frac{\mu_{\text{g}}}{2} \left[\frac{4}{3} - \frac{5,58-3,82}{2} \right] = 0,373 \mu_{\text{яд}}$ - для случая jj-связи.
Решени е. Нецентральность ядерных сил ведет к несохранению момента импульса, поэтому основное состояние не есть чистое s-состояние ($L = 0$), а содержит также примесь состояния с $L = 2$ (D-состояние). На-

личие только четных моментов - следствие закона сохранения четности. Что же касается полного момента J, то он всегда является интегралом движения. Поэтому $J = 1$ в обоих случаях. Параллельность спинов (при этом $S = 1, 2S + 1 = 3$) - экспериментальный факт, и с $S = 0$ связанного состояния нет.

Заметим, что при реализации ls-связи полный момент $\mathbf{J} = \mathbf{L} + \mathbf{S}$, где $\mathbf{L} = \sum_i \mathbf{1}_i; \mathbf{S} = \sum_i \mathbf{s}_i$. При реализации jj-связи $\mathbf{J} = \sum_i \mathbf{j}_i$, где $\mathbf{j}_i = \mathbf{1}_i + \mathbf{s}_i$.

Для дейтрона в состоянии $^3D_1 : L = 2; S = 1$; g-факторы протона и нейтрона: $g_{l\text{p}} = 1$; $g_{l\text{n}} = 0$ (поскольку заряд равен нулю); $g_{\text{sp}} = 5,58$; $g_{\text{sn}} = -3,82$. Если $\mathbf{L}$ - орбитальный момент дейтрона, а $\mathbf{S}$ - спиновый, то в силу зарядовой независимости p и n для ядерных сил $\mathbf{1}_{\text{p}} = \mathbf{1}_{\text{n}} = \mathbf{L}/2$; $s_p = s_n = \mathbf{S}/2$. Таким образом, можно записать:

$$\mu_{\text{d}} = \left(g_{l\text{pp}} \mathbf{1}_{\text{p}} + g_{sp} \mathbf{s}_{\text{p}} + g_{\text{sn}} \mathbf{s}_{\text{n}} \right) \mu_{\text{gд}} = \left[\frac{\mathbf{L}}{2} + \left(g_{sp} + g_{sn} \right) \frac{\mathbf{s}}{2} \right] \mu_{\text{яд}}$$

Далее надо вычислить проекцию вектора μ_d на направление , которая и называется магнитным моментом дейтрона в ls-связи

$$\mu_{\mathrm{d}} = \frac{\mu_{\mathrm{gn}}}{2}\left[\langle \mathbf{L}\cos(\mathbf{LJ})\rangle + (g_{sp}+g_{sn})\,\langle \mathbf{S}\cos(\mathbf{SJ})\rangle\right]$$

Здесь $\langle \mathbf{LJ}\rangle = \langle LJ\cos(\mathbf{LJ})\rangle$, откуда $\langle L\cos(\mathbf{LJ})\rangle = \frac{\langle \mathbf{LJ}\rangle}{J}\frac{J}{J} = \frac{\langle J(\mathbf{LJ})\rangle}{J^2}$. К роме того, $\langle \boldsymbol{S}\cos(\mathbf{SJ})\rangle = \frac{\langle J(\mathbf{SJ})\rangle}{J^2}$. Подсчитаем:

$$\langle L\cos(\mathbf{L})\rangle = J\frac{J(J+1)+L(L+1)-S(S+1)}{2J(J+1)} = \frac{1}{4}[2+6-2] = \frac{3}{2}$$

$$\langle S\cos(\mathbf{SJ})\rangle = \frac{J}{2J(J+1)}[J(J+1)+S(S+1)-L(L+1)] = -\frac{1}{2}$$

Отсюда и следует первый ответ: $\mu_d^{(1)} = 0,31\mu_{\text{яд}}$.
Что же касается магнитного момента дейтрона при реализации jj-связи, то в этом случае подсчет следует осуществлять так:

$$\langle \boldsymbol{\mu}\rangle = \langle g_{\mathbf{n}}\mu_{\boldsymbol{g}}\mathbf{j_n} + g_{\mathrm{p}}\mu_{\boldsymbol{gj}}\mathbf{j}_{\mathrm{p}}\rangle = g\mu_{\text{яд}}\,\mathbf{J}$$

При этом

$$g = g_{\mathrm{n}}\frac{\langle \mathbf{j}_{\mathrm{n}}\mathbf{J}\rangle}{2J^2} + g_{\mathrm{p}}\frac{\langle \mathbf{j}_{\mathrm{p}}\mathbf{J}\rangle}{2J^2} = \frac{g_{\mathrm{n}}+g_{\mathrm{p}}}{2}$$

Определим g-факторы протона и нейтрона g_{p} и g_{n}. Имеем

$$\langle \mu_{\mathbf{n}}\rangle = g_{\mathbf{n}}\mu_{\text{я}}\,\mathbf{j_n},\ \text{где}\ \mu_{\mathbf{n}} = g_{\boldsymbol{sn}}\mu_{\text{я}}\,\mathbf{s_n}$$

Умножая оба выражения на $\mathrm{j_n}$ и усредняя при этом скалярное произведение, получим

$$\langle \mu_{\mathrm{n}}\mathrm{j_n}\rangle = g_{\mathrm{n}}\mu_{\mathrm{g}}\left\langle \mathrm{j}_{\mathrm{n}}^2\right\rangle = g_{sn}\mu_{\text{gд}}\ \langle \mathbf{s}_n\mathrm{j}_n\rangle\,,\ \text{откуда следует, что}$$

$$g_{\mathrm{n}} = \frac{\langle \mathbf{s}_{\mathrm{n}}\mathrm{j_n}\rangle}{\langle \mathrm{j}_n^2\rangle}g_{sn} = g_{\mathrm{sn}}\frac{s_{\mathrm{n}}\left(s_{\mathrm{n}}+1\right)+j_{\mathrm{n}}\left(j_{\mathrm{n}}+1\right)-l_{\mathrm{n}}\left(l_{\mathrm{n}}+1\right)}{2j_{\mathrm{n}}\left(j_{\mathrm{n}}+1\right)} = -\frac{g_{sn}}{3} = \frac{3,82}{3}.$$

Совершенно аналогично опеределяется и протонный g-фактор:

$$g_{\mathrm{p}} = \frac{\langle \mathrm{I_p j_p}\rangle}{\left\langle \mathrm{j}_{\mathrm{p}}^2\right\rangle} + g_{sp}\frac{\langle\ \mathrm{s_p j_p}\rangle}{\left\langle \mathrm{j}_{\mathrm{p}}^2\right\rangle} = \frac{4}{3} - \frac{5,58}{3}$$

Подставив результаты для g_{n} и g_{p}, получим ответ

$$g = \frac{g_{\mathrm{n}}+g_{\mathrm{p}}}{2} = 0,373,\ \text{т. е.}\ \mu_{\mathrm{d}}^{(2)} = 0,373\mu_{\text{мд}}$$

Поскольку обе модели дают близкие результаты, то отдать предпочтение какой-то из них на основе экспериментальных данных невозможно (см. задачу 7.61).

7.

61. $w = 0,035(3,5\%)$ (см, также замечание в начале решения задачи 7.60). Если обозначить искомую вероятность как w, то тогда средний магнитный момент дейтрона, измеряемый в опыте, есть

$$\langle \mu\rangle = (1-w)\mu\left({}^3S_{\mathrm{I}}\right) + w\mu\left({}^3D_{\mathrm{I}}\right)$$

откуда и следует приведенный ответ.

7.

62. $\delta\varrho_{\text{допл}} = \frac{Q\mathscr{E}_\gamma}{Mc^2} = 5,7$ В; $\quad \delta\varrho_{\text{отд}} = \frac{\mathscr{E}_y^2}{2Mc^2} = 2,5$ В; $\quad \delta\mathscr{E}_0 \approx \frac{\hbar}{\tau_1} + \frac{\hbar}{\tau_2} \approx \approx \frac{\hbar}{\mathrm{T}_1} = 2\cdot 10^{-2}$ В.

7.

63. Амплитуда сигнала ЯМР пропорциональна количеству соответствующих ядер. Поэтому первый пик соответствует ЯМР на ядрах трития. $\mu(\mathrm{t}) = \frac{h\nu I}{B_1} = 2,97\mu_{\text{яд}} = 1,5 \cdot 10^{-23}$ эрг/с, где $I = \frac{1}{2}.\mu(t) - \mu_{\text{теор}}\,(\mathrm{t}) = (2,97 - 2,79)\mu_{\text{яД}} = 0,18\mu_{\text{яд}}$.

7.

64. $\Delta\mu_{\text{He}} = |\mu_{\text{эксп}} - \mu_{\text{теор}}| = 0,22\mu_{\text{яд}} = 0,11 \cdot 10^{-23}$ эрг /, где $\mu_{\text{эксп}} = -2,13\mu_{\text{яд}}$; $\mu_{\text{теор}} = -1,91\mu_{\text{яд}}$.

7.

65. $R_m = \frac{hc}{\varrho \sin\theta_m}, m = 1,2,3; R_{\text{ср}} = 3,5 \cdot 10^{-13}$ cm. $(r_0)_{\text{ср}} = \frac{R_{\text{ср}}}{AV^3} \approx 1,2.$

18.2.4 Problems about neutrons 1

O3.1-8.1

Нейтрон упруго рассеивается на ядре. Какое минимальное отличное от нуля прицельное расстояние b может реализоваться для нейтрона с энергией $\mathscr{E} = 100$ кэВ (рис. 46)?

8.

1. По закону сохранения момента импульса $bp = L = \hbar\sqrt{l(l+1)}$. Минимальное значение $l = 1$, откуда $b_{\min} = \frac{\hbar\sqrt{2}}{p} = \frac{\hbar\sqrt{2}}{\sqrt{2\ \mathrm{m}\ \S}} = \frac{\hbar}{\sqrt{\mathrm{m}}} = 2 \cdot 10^{-12}$с.

O3.1-8.2

Оценить отношение сечений образования компаунд-состояния (составного ядра) при бомбардировке ядер $^{40}_{20}$Ca нейтронами и протонами с одной и той же начальной энергией $\mathscr{E}_0 = 10$МВ.

8.

2* $\frac{\sigma_c(p)}{\sigma_c(n)} \approx 0,5.$

Решение. Рассмотрим сначала случай рассеяния нейтрона на ядре (рис. 179). Возможные значения прицельных расстояний b_l определяются из правила квантования момента импульса

$$pb_l = \hbar\sqrt{l(l+1)}$$

Импульс нейтрона $p = \hbar/\lambda$. В квазиклассическом приближении ($l \gg 1$) $b_l \approx l$. Разобьем пространство, занимаемое падаюuим пучком нейтронов, на кольцевые зопы, ширина которых равна λ. В каждой из этих зон будут двигаться частицы с определенным значением момента импульса. Число ча стиц в такой зоне (при условии их равномерного распределения в простран стве) пропорционально площади кольца со средним радиусом b_l

$$S_l = \frac{1}{2}\pi\left(b_{l+1}^2 - b_{l-1}^2\right) = \pi\hbar^2(2l+1).$$

Полученная величина S_l - это геометрическое сечение, пропорциональное доле всех частиц, имеющих квантовое число l, из всего потока падающих на ядро нейтронов. Умножая S_l на вероятность

w_l поглощения ча-

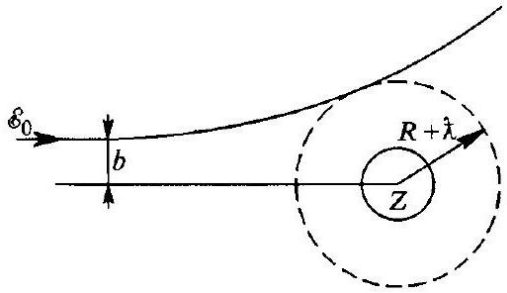


Рис. 179 стицы ядром, получим парциальное сечение образования составного ядра для частицы с моментом l.

Вероятность поглощения зависит от внутренних свойств ядра и от характеристики сил, действующих на частицу вне ядра. В общем случае она пропорциональна вероятности проникновения через кулоновский и центробежный барьеры. Конечно, существует отражение и при $l = 0$.
Представим w_l в виде

$$w_l = P_l \zeta_l,$$

где P_l - вероятность проникновения через внешний барьер, ζ_l - вероятность «прилипания» частицы к ядру. Тогда полное сечение поглощения (образования составного ядра), включая случай с $l = 0$, есть

$$\sigma_{\mathrm{c}}(\mathrm{n}) = \sum_{l=0}^{\infty} (2l+1)\pi \hat{\lambda}^2 P_l \zeta_l.$$

Чтобы ядро поглотило частицу, она должна попасть в область действия ядерных сил, т.е. $(b_l)_{\max} \leqslant R$, откуда $l_{\max} \approx R/\lambda$. Что касается величины ζ_l, то будем считать, что ядро поглощает все падающие на него частицы (модель черного ядра). Тогда $\zeta_l = 1$ при $l \leqslant R/\lambda$ и

$$\sigma_{\mathrm{c}}(\mathrm{n}) = \sum_{l=0}^{R/\lambda} (2l+1)\pi \hbar^2 P_l$$

В области энергий нейтронов порядка нескольких МэВ и выше, когда $\lambda \ll R$, можно считать, что $P_l \simeq 1$, и тогда

$$\sigma_{\mathrm{c}}(\mathrm{n}) = \sum_{l=0}^{R/\lambda} (2l+1)\pi \lambda^2 = \pi (R+\lambda)^2$$

В случае рассеяния протонов составное ядро образуется лишь тогда, когда энергия протона будет больше кулоновского барьера (туннельным эффектом при данной энергии можно пренебречь). Для вычисления воспользуемся полученным выше результатом (*). Как видно из этой формулы, эффективный размер ядра стал равным $R+\lambda$. Пусть на бесконечности энергия и прицельное расстояние протона равны $\mathscr{E}_0$ и b. Тогда закон сохранения энергии дает уравнение (в системе центра инерции)

$$\mathscr{E} = \mathscr{E}_0 - \frac{Ze^2}{R+\hbar}$$

Соответствующий закон сохранения момента импульса -

$$b\sqrt{2m\wp_0} = (R+\lambda)\sqrt{2m\complement^\circ}$$

откуда сразу следует предельное значение b:

$$b = (R+\lambda)\sqrt{\frac{\varrho}{\varrho_0}}$$

Тогда искомое сечение образования составного ядра под действием протонов

$$\sigma_{\mathrm{c}}(\mathrm{p}) = \pi b^2 = \pi (R+\hat{\lambda})^2 \frac{\mathscr{E}}{\mathscr{E}_0} = \pi (R+\lambda)^2 \left[1 - \frac{Ze^2}{\varrho_0 (R+\hbar)}\right].$$

Отношение сечений

$$\frac{\sigma_c(\mathrm{p})}{\sigma_{\mathrm{c}}(\mathrm{n})} = 1 - \frac{Ze^2}{\varrho_0 (R+\hbar)} \approx \frac{1}{2}$$

где $\hat{\lambda} = \frac{\hbar}{\sqrt{2}\ _0} = 1,5 \cdot 10^{-13}$ cm; $R_{\mathrm{Ca}} = 1,3 \cdot 10^{-13} A^{1/3} = 4,45 \cdot 10^{-13}$ cm (величины соизмеримые).

О3.1-8.3

Оценить полное сечение σ взаимодействия ультрарелятивистского нейтрона с ядром урана. Приняв для сечения нуклон-нуклонного взаимодействия величину $\sigma_{\mathrm{NN}} \approx 40$ мбн, оценить длину свободного пробега такого нейтрона в ядре.

8.

3. $\sigma_{\text{полн}} = 2\pi R_{\mathrm{U}}^2 \approx 4,1$ бн. В релятивистском случае дебройлевская длина волны $t = \hbar/p \leq \hbar/(m_{\mathrm{n}}c) = 2 \cdot 10^{-14}$ см, что много меньше $R_{\mathrm{U}} \approx \approx 8 \cdot 10^{-13}$ cm. Таким образом, сечение поглощения неупругого рассеяния $\sigma_{\text{погл}} = \pi (R_{\mathrm{U}} + \lambda)^2 \approx \pi R_{\mathrm{U}}^2$, т. е. все частицы с прицельным расстоянием, меньшим R_{U}, выбывают из пучка и поглощаются. Ядро ведет себя как поглощающий шар (модель «абсолютно черного ядра»). Действительно, длина пробега нуклона $l = \frac{1}{\sigma_{\mathrm{NN}} n} = \frac{4\pi r_0^3}{3\sigma_{\mathrm{NN}}} \approx 2 \cdot 10^{-13}$ см $\ll R_{\mathrm{U}}$. Однако из-за дифракции на краю ядра происходит отклонение частиц от первоначального направления - упругое рассеяние. Согласно принципу Бабине для дифракции Фраунгофера количество света, рассеянного на черном теле, равно количеству света, падающего на него и поглощаемого им, $\sigma_{\text{погл}} = \sigma_{\text{диф}}$. Следовательно, $\sigma_{\text{полн}} = \sigma_{\text{погл}} + \sigma_{\text{диф}} = 2\sigma_{\text{погл}}$ (дифракционное удвоение), поэтому $\sigma_{\text{полн}} = 2\pi R_{\mathrm{U}}^2 \approx 4,16$Н.

О3.1-8.4

Медленный нейтрон упруго рассеивается на свободном ядре со спином $I = 3/2$ в состоянии с орбитальным моментом $L = 0$. Определить вероятность рассеяния в состояниях с параллельной и антипараллельной взаимной ориентацией спинов нейтрона и ядра.

У к з з н и е.

Учесть, что ядерные силы между нуклонами зависят от взаимной ориентации их спинов и поэтому сечение рассеяния зависит от полного углового момента сталкивающихся частиц, являЮщегося интегралом движения. Спином ядра называют его полный момент. В данном случае (при $L = 0$) спин ядра является «чистым» спином в традиционном его понимании.

8.

4: Вероятность рассеяния с параллельной ориентацией спинов $\frac{I+1}{2I+1} = \frac{5}{8}$, а с антипараллельной $\frac{I}{2I+1} = \frac{3}{8}$.

Решение. Для медленных частиц минимальное прицельное расстояние (см. задачу 8.1) много больше размеров ядра, и поэтому реакция возможна только при $l = 0$. Таким образом, полный момент является чисто спиновым, и число спиновых состояний системы из двух частиц есть $(2S + 1)(2I + 1) = 2(2I + 1)$. При этом полный момент (спин) может принимать два значения: $I + 1/2$ и $I - 1/2$. Первому моменту соответствует $2(I + 1/2) + 1 = 2(I + 1)$ значений проекции момента, второму $2(I - 1/2) + 1 = 2I$.

Вероятность рассеяния пропорциональна относительной доле состояний с заданной проекцией полного момента, т. к. энергия взаимодействия не зависит от значения проекции.

О3.1-8.5

Вплоть до энергий $T = 20$ МэВ угловое распределение рассеянных нейтронов в реакции пр $\to$ пр в лабораторной системе отсчета хорошо описывается формулой $d\sigma(\theta) = A \cos\theta d\Omega$. Как выглядит это распределение в системе центра инерции? Какая оценка для радиуса действия ядерных сил отсюда следует?

8.

5. $\frac{d\sigma_{\text{наб}}}{d\Omega} = \frac{d\sigma_\mu(\theta')}{d\Omega'}$; $\theta' = 2\theta; d\sigma_\mu = \frac{A}{4} d\Omega'$, т. е. нейтроны в системе центра масс (СЦМ) рассеиваются изотропно. $R \approx \hbar \approx 10^{-13}$ см. Полученные формулы следуют из векторных диаграмм рассеяния в ЛСО и СЦМ.

Приведем для сведения формулу для пересчета дифференциального сечения из «Л» - лабораторной системы в «ЦМ» - систему центра масс в общем виде

$$\left(\frac{d\sigma(\theta)}{d\Omega}\right)_{\mathrm{J}} = \left(\frac{d\sigma(\theta')}{d\Omega}\right)_{\mathbf{LM}} \frac{\left(m_1^2 + 2m_1 m_2 \cos\theta' + m_2^2\right)^{3/2}}{m_2^2 (m_2 + m_1 \cos\theta')}$$

где штрихом обозначены углы в СЦМ, m_2 - покоящаяся масса, m_1 - движушаяся.

О3.1-8.6

Тепловой нейтрон из реактора попадает по нормали в биологическую защиту (рис. 47), состоящую в основном из водорода (например, парафин), толщиной $l = 1$ m и плотностью ядер $n = 10^{22}\text{см}^{-3}$. Сечение упругого рассеяния составляет $\sigma_{\text{расс}} = \sigma_0 = 20$ бн, сечение поглощения $-\sigma_{\text{погл}} = \sigma_1 = 0,3$ бн и не зависит от энергии. Угловое распределение упруго рассеянных нейтронов в системе центра масс изотропно. Считая, что после рассеяния нейтрон пролетает в защите путь в $1/\cos\theta$ раз больший, чем при прямом пролете, где θ - угол рассеяния, оценить вероятность того, что нейтрон пройдет через защиту, испытав лишь только одно упругое столкновение [l].

8.

6.* $w \approx 4 \cdot 10^{-9}$. Решение. Уменьшение потока нейтронов связано с актами захвата и рассеяния. Так, в слое защиты толщиной dx, находящемся на расстоянии x от места входа нейтронов, их поток уменьшится на величину

$$dj = -j(x)\frac{dx}{\lambda}$$

где $\lambda \approx \frac{1}{n\sigma_{\text{полн}}}$ - длина свободного пробега нейтрона. Полное сечение реакции (как захват, так и упругое рассеяние) $\sigma_{\text{полн}} = \sigma_{\text{погл}} + \sigma_{\text{расс}} \approx \sigma_{\text{расс}} = \sigma_0$. Таким образом,

$$j(x) = j_0 e^{-n_{\sigma_0} x}$$

где j_0 - поток нейтронов на входе. Перепишем это выражение в дифференциальной форме

$$dj = -j_0 n\sigma_0 e^{-n_{\sigma_0} x} dx$$

Таким образом вероятность упругого рассеяния нейтрона в слое толщиной dx на расстоянии x от входа в защиту

$$dw = \left|\frac{dj}{j_0}\right| = n\sigma_0 e^{-n_0 x} dx$$

После столкновения нейтроны проходят путь $\frac{l-x}{\langle\cos\theta\rangle}$. Определим среднее значение косинуса угла рассеяния, имея в виду замечание в условии задачи, что в системе центра масс угловое распределение упруго рассеянных нейт-
ронов изотропно. Как показано в предыдущей задаче 8.5, в этом случае в лабораторной системе отсчета $d\sigma(\theta) = A\cos\theta d\Omega$. Таким образом,

$$\langle\cos\theta\rangle = \frac{\int_0^{\pi/2}\cos\theta\cos\theta d\Omega}{\int_0^{\pi/2}\cos\theta d\Omega} = \frac{\int_0^{\pi/2}\cos^2\theta d(\cos\theta)}{\int_0^{\pi/2}\cos\theta d(\cos\theta)} = \frac{2}{3}.$$

Вероятность выйти из защиты без какого-либо взаимодействия после рассеяния в точке, находящейся на расстоянии x от места входа,

$$dw(x) = n\sigma_0 e^{-n\sigma_0 x} dx \exp\left(-n\sigma\frac{l-x}{\langle\cos\theta\rangle}\right)$$

Искомая вероятность пройти защиту, испытав лишь одно упругое столкновение,

$$w = \int_0^l n\sigma_0 e^{-n_{\sigma_0}x} e^{-n_{\sigma_0}\frac{3}{2}(l-x)} dx = n\sigma_0 e^{-\frac{3}{2}n_{\sigma_0}l}\int_0^l e^{\frac{1}{2}n_{\sigma_0}x} dx \approx 2e^{-20} = 4\cdot 10^{-9}.$$

О3.1-8.7

Плотность потока нейтронов, выходящих из реактора, равна $j_0 = 10^{14}\text{с}^{-1}\cdot\text{см}^{-2}$. Определить выход реакции в единицу времени (отношение числа актов реакции к числу частиц, упавших на единицу площади мишени в единицу времени) в мишени толщиной 1см. Сечение реакции $\sigma = 10^{-27}\text{см}^2$, плотность ядер мишени $n = 10^{22}\text{см}^{-3}$.

О3.1-8.8

Узкий пучок тепловых нейтронов проходит через слой воды толщиной 1 см. Определить доли первоначального потока нейтронов, выбывающих из пучка в результате поглощения и рассеяния. Сечение поглощения для воды $\sigma_{\text{погл}} = 0,66$ бн, а сечение рассеяния $\sigma_{\text{расс}} = 696$Н.

8.

7. $\frac{j_0-j_d}{j_0} \approx n\sigma d = 10^{-5}$.

8.

8. $\alpha_{\text{расс}} = 0,9; \alpha_{\text{погл}} = 0,022$.

О3.1-8.9

Определить, во сколько раз уменьшается интенсивность узкого пучка тепловых нейтронов после прохождения пластинки Al толщиной $d = 3$ см. На выходе из пластинки регистрируется пучок первоначальной ширины. Сечение рассеяния для алюминия $\sigma_{\text{расс}} = 1,41$ бн, а сечение поглощения $\sigma_{\text{погл}} = 0,23$ бн.

8.

9. $\frac{j_0}{j} = \exp\left(\frac{d\rho N_{\text{A}}\sigma}{A}\right) \approx 1,35$, где $\sigma = \sigma_{\text{расс}} + \sigma_{\text{погл}} = 1,64$ бн.

О3.1-8.10

Быстрые нейтроны, попав в воду, быстро замедляются до тепловых скоростей $v = 2,2$ km/c и диффундируют в ней, пока не захватятся ядрами водорода (захватом кислородом можно пренебречь). Оценить время жизни т нейтронов в воде. Сечение захвата (поглощения) теплового нейтрона протоном $\sigma_{\text{погл}} = \sigma = 0,3$ бн.

8.

10. $\tau = \frac{\mu}{2\rho N_{\text{A}}\sigma\nu} = 2,3 \cdot 10^{-4}$ с. Отметим, что в области справедливости закона Бете $\alpha = \sigma_{\text{погл}} \propto 1/v$, время жизни нейтрона в среде не зависит от его энергии.

О3.1-8.11

Исследование структуры жидкого или твердого ^{3} He с помощью пропускания нейтронов через слой вещества затруднено из-за большой величины сечения экзотермической реакции $^3\text{He}(\text{n},\text{p})^3\text{H}$, и для нейтронов с энергией 300 K оно равно $\sigma_0 = 5400$ бн. Определить энергию нейтронов, с помощью которых можно изучать слои ^{3} He толщиной $d = 1$ мм, чтобы проходило не менее 10% от потока падающих нейтронов. Концентрация ядер ^{3} He $n = 10^{22}$см$^{-3}$.

Ук а з а н и е. Сечение указанной реакции для нейтронов с энергией до 1 МэВ имеет нерезонансный характер.

8.

11. $\mathscr{E} = \mathscr{E}_0\left(\frac{\sigma_0 nd}{\ln(j_0/j)}\right)^2 \approx 0,14$ эВ, где $\mathscr{E}_0 = 0,025$ эВ.

О3.1-8.12

Для регистрации медленных нейтронов широко используются счетчики, наполненные газообразным изотопом ^{3} He. Рассчитать долю ε регистрируемых частиц - эффективность счетчика,

представляющего собой цилиндр диаметром $d = 25$ мм, наполненный газом при давлении $P = 10$ атм. Нейтроны при температуре $T = 300$ K летят вдоль диаметра цилиндра. В счетчике происходит реакция $^3\text{He}(\text{n},\text{p})^3\text{H}$, сечение которой для регистрируемых нейтронов $\sigma = 5400$ бн.

О3.1-8.13

Для детектирования медленных нейтронов широко используются ионизационные счетчики, наполненные ^{3}He. Регистрация нейтронов производится по реакции $\left(\mathrm{n}, {}^3\mathrm{He}\right) \rightarrow \left({}^3\mathrm{H}, \mathrm{p}\right)$. Показать на основе законов сохранения, что взаимодействие нейтронов с гелием-3 не может приводить к образованию ^{4} He по реакции $\mathrm{n} + {}^3\mathrm{He} \rightarrow {}^4\mathrm{He}$.Cm. также задачу 1.16.

О3.1-8.14

В сечении рассеяния нейтронов на ядрах может проявляться «волновой резонанс», когда интерференция нейтронных волн де Бройля приводит к «прозрачности» чдер (ядерный аналог эффекта Рамзауэра). Оценить, при какой минимальной энергии нейтронов должны быть видны Эти «резонансы проницаемости» на ядре ^{208} Pb. Ядерный потенциал считать одномерной ямой, ширина которой равна диаметру ядра, глубина ямы $U = 40\mathrm{M} \ni \mathrm{B}$ (см. задачу 3.33).

О3.1-8.15

Источник тепловых нейтронов установлен в центре большого графитового куба, и со временем нейтроны, многократно рассеиваясь на ядрах углерода и иногда поглощаясь, распространяются по всему объему. Оценить эффективный размер области, занимаемой в результате нейтронами, если эффективное сечение рассеяния нейтронов $\sigma_{\text{расс}} = 4,8 \cdot 10^{-24}\text{см}^2$, а поглощения $-\sigma_{\text{погл}} = 3 \cdot 10^{-27}\text{см}^2$. Плотность графита $\rho = 2,2$ г/ cm^3.

О3.1-8.16

Поликристаллический бериллий слабо поглощает, но интенсивно рассеивает нейтроны (брэгговское отражение на кристалликах). На этом основано действие поликристаллического фильтра, пропускающего нейтроны с энергией $\mathcal{E} < \mathscr{E}_{\text{гр.}}$. Найти $\sigma_{\text{гр}}$ для бериллия, у которого межплоскостное расстояние $d = 2\text{Å}$.

О3.1-8.17

Поток нейтронов из реактора, имеющих максвелловское распределение по скоростям с температурой $T = 370$ K, пропускается через толстый поликристаллический фильтр из спрессованного порошка графита. Найти. какая поля нейтпонов ппохолит чепез такой фильтр. Максимальное межплоскостное расстояние для решетки графита $a = 3,35\text{Å}$.

О3.1-8.18

Два цилиндрических стержня с одинаковыми диаметрами, один из графита, другой из висмута, совмещены основаниями. Графитовый стержень через открытый торец облучается параллельно его оси потоком нейтронов, выходящих из замедлителя с комнатной температурой 300 K (рис. 48). Полагая рассеяние нейтронов в графите и висмуте брэгговским, оценить, во сколько раз средняя кинетическая энергия нейтронов $\mathcal{E}_k$, выходящих из висмутового цилиндра через его боковую поверхность, меньше энергии падающих нейтронов $\mathcal{E}_0$. Максимальное 71 расстояние между кристаллическими плоскостями для графита $d_{\text{c}} = 3,35\text{Å}$ и для висмута $d_{\text{Bi}} = 4,05\text{Å}$. Длина стержней много боль ше их диаметров, которые сравнимы со средним пробегом нейтронов.

8. SOLUTIONS Нейтроны. Ядерные реакции

8.

12. $\varepsilon = 1 - \exp\left(-\frac{P \circ d}{kT}\right) \approx 96\%$.

8.

13* Решение. Энергия связи ^{3} Не равна 7,7 МэВ, а ^{4}He – 28,3 МэВ, т. е. реакция в принципе экзотермическая. Однако трехчастичная реакция невозможна, как это имеет место при фотоэффекте на свободном электроне, в силу законов сохранения энергии и импульса

$$\begin{cases} \frac{mv^2}{2} + Q = \frac{MV^2}{2}; \\ mv = MV \end{cases}$$

Поскольку $M \approx 4m$, то $v = 4V$. Тогда

$$16V^2 + \frac{2Q}{m} = 4V^2, \quad 5V^2 + \frac{Q}{m} = 0.$$

Из последнего равенства видно, что реакция невозможна при $Q > 0$.

8.

14. Условие резонанса $2R_{\text{Я}} = n\frac{\lambda}{2} = \frac{n\pi\hbar}{\sqrt{2m_N(\mathscr{G}_n+U)}}, \mathscr{E}_n > 0$ (энергия отсчитывается от потолка ямы), откуда $n^2 \cdot 0,864$ МэВ $> U$. Минимальное целое n, которое удовлетворяет этому условию, есть $n = 7$, при этом $\mathfrak{E}_n = 2,34$М эВ.

8.

15: $L_{\text{эфф}} = \frac{A}{\rho N_{\text{A}}\sqrt{3\sigma_{\text{расс}}\,\sigma_{\text{погл}}}} \approx 44$ cm.

Решение. Длина свободного пробега частицы $\lambda = \frac{1}{n\sigma}$. В данном случае существуют два механизма взаимодействия нейтронов с ядрами углерода рассеяние и поглощение (захват). Следовательно, имеются две длины свободного пробега. Время пробега до захвата $t_{\text{погл}} = \frac{\lambda_{\text{погл}}}{v}$. Искомый эффективный размер области, занимаемой нейтронами, определяется временем $t_{\text{погл}}$

$$L_{\text{эфф}} = \sqrt{6Dt_{\text{пог}}}$$

где коэффициент диффузии D в свою очередь определяется рассеянием нейтронов, т. е. $D = (1/3)\lambda_{\text{расс}}\, v$. Подстановкой получим

$$L = \sqrt{2\lambda_{\text{расс}}\, v \cdot \frac{\lambda_{\text{погл}}}{v}} = \sqrt{2\lambda_{\text{погл}}\,\lambda_{\text{расс}}} = \left(\frac{n^2\sigma_{\text{погл}}\,\sigma_{\text{расс}\,2}\right)^{-1/2} \ldots .}{2}.$$

Плотность атомов углерода $n = \rho N_{\text{A}}/A$. Таким образом,

$$L_{\text{эфф}} = \frac{A\sqrt{2}}{\rho N_{\text{A}}\,(\sigma_{\text{расс}}\,\sigma_{\text{погII}}\,)^{1/2}} \approx 107 \text{ cm}.$$

8.

16. Условие пропускания: $\lambda > 2d$, где λ - длина волны де Бройля для бериллия. Отсюда $\mathscr{E}_{\mathbf{r}\rho} = \frac{\pi^2\hbar^2}{2md^2} \approx 5 \cdot 10^{-3}$ эВ .

8.

17. $\alpha = \frac{1}{2}\left(\frac{\pi^2\hbar^2}{2m_{\text{n}}kTa^2}\right)^2 = 0,16\%$.

8.18. $\frac{\mathscr{E}_{\text{C}}}{\mathscr{E}_{\text{к}}} = \frac{2kT}{(\mathscr{E}_{\text{C}}+\mathscr{E}_{\text{Bi}})/2} \approx 34$, где $\mathscr{E}_{\text{C}} = \frac{\hbar^2}{2m\lambda_{\text{C}}^2}$; $\mathscr{E}_{\text{Bi}} = \frac{\hbar^2}{2m\lambda_{\text{Bi}}^2}$, а $\lambda_{\text{C}} \geqslant 2d_{\text{C}}$ и $\lambda_{\text{Bi}} \geqslant 2d_{\text{Bi}}$ (нейтроны с длинами волн от λ_{C} до λ_{Bi} рассеиваются в висмуте и выходят через его поверхность).

8.

19. $v_{\text{r}\rho} = \frac{2\hbar\sqrt{-\pi Nf}}{m_{\text{r}}}$ при условии, что $f < 0$.

8.

20. $\varphi_0 \approx \sqrt{1-n^2} = \lambda\sqrt{-\frac{Nf}{\pi}}$.

8.

21. $1-n^2=-\frac{2\pi\hbar^2\rho N_{\text{A}}f}{m_{\text{n}}{}'A}=1,23\cdot10^{-5},\theta\approx\sqrt{1-n^2}\approx12'$ (угол скольжения).

8.

22. $f=-\frac{\pi}{N\lambda^2}=-\frac{m_n^2v^2A}{4\pi\hbar^2\rho N_{\text{A}}}\approx-0,78\cdot10^{-12}$ cm.

8.

23. Сечение упругого рассеяния нейтронов $\sigma=-\frac{\ln0,7}{n_{\text{m}}d}=5,45$ бн, где $n_{\text{m}}=\rho N_{\text{A}}/A_{\text{Pb}}$ - концентрация ядер мишени. При упругом s-рассеянии $\sigma=4\pi|f|^2$, откуда $R_{\text{я}}=\sqrt{\frac{\sigma}{4\pi}}=6,6\cdot10^{-13}$ см. Доказательство того, что происходит s-рассеяние, т. е. рассеяние с нулевым моментом импульса, основано на подсчете квантового числа l в условии $pR_{\text{я}}=\sqrt{2m_n\S}R_{\text{я}}=\hbar\sqrt{l(l+1)}$, откуда $l\simeq0,4$, т. е. в самом деле преобладает s-рассеяние.

8.

24. $H=\left(\frac{3nh}{4m\sqrt{2g}}\right)^{2/3}\approx0,034$ mm.

8.

25. $f=-\frac{gHAm_{\text{n}}^2}{2\pi\hbar^2\rho N_{\text{A}}}\approx-8,4\cdot10^{-13}$с.

8.

26*. Решение. Скорость счета, т. е. число нейтронов, попавших в детектор в единицу времени, есть произведение плотности потока нейтронов j на площадь детектора. Поскольку распределение нейтронов в реакторе максвелловское, то

$$dj(v)=vdn(v)=Av\cdot v^2\exp\left(-\frac{mv^2}{2kT}\right)dv$$

где A - нормировочная постоянная.
Для ультрахолодных нейтронов $\frac{mv^2}{2k}=T^*=6\cdot10^{-3}$ K $\ll T$, поэтому с хорошей точностью экспоненту можно считать равной 1. Тогда $dj(v)=Av^3dv=A'\mathscr{E}d\mathscr{E}$, где $\mathscr{E}=mv^2/2$. При «падении» нейтронов вниз их скорость увеличивается и может превысить граничное значение $v_{\text{гр}}$, вследствие чего такой нейтрон покинет трубу и не попадет в счетчик. Предельная энергия $\mathscr{E}'=\mathfrak{E}-mgH=\frac{mv_{\text{гр}}^2}{2}-mgH$. Суммарная плотность потока нейтронов

$$j=A'\int_0^{\mathfrak{E}'}\mathscr{E}d\mathscr{E}=\frac{A'}{2}\mathfrak{E}'^2=\frac{A'}{2}\left(\frac{mv_{\text{гр}}^2}{2}-mgH\right)$$

Счет прекратится при $\mathscr{E}'=0$, откуда предельное значение

$$H=\frac{v_{\text{гр}}^2}{2g}=5\text{ m}$$

8.

27. $j\propto\left(\frac{mv_{\text{гр}}^2}{2}-mgH\right);H_{\text{гр}}=\frac{v_{\text{гр}}^2}{2g}=5$ m.

8.

28. $S = \frac{4V}{v\tau} = 0,8 \text{ mm}^2$.

8.

29. $\alpha = \sqrt{\frac{6}{\pi}}(\sin i)^3 = 3,4 \cdot 10^{-8}$.

8.

30*. $j \approx 18900$ нейтронов/с.

Решение. Чтобы понять, как ведут себя нейтроны с заданной энергией $\mathscr{E} = 10^{-7}$ эВ в меди и алюминии, вычислим длину волны таких нейтронов:

$$v = \sqrt{\frac{2\mathscr{E}}{m}} = 4,38 \text{ m/c}; \quad \lambda = \frac{h}{mv} = 9,05 \cdot 10^{-6} \text{ cm}.$$

Предельные длины волн для нейтронов в меди и алюминии

$$\lambda_{\mathbf{r}\rho} = \sqrt{\frac{\pi}{N|f|}} = \sqrt{\frac{\pi A}{\rho N_{\text{A}}|f|}} = \begin{cases} 6,9 \cdot 10^{-6} \text{ cm(Cu)}, \\ 12,2 \cdot 10^{-6} \text{ cm(Al)}. \end{cases}$$

Таким образом, длина волны нейтронов данной энергии удовлетворяет неравенству

$$\lambda_{\Gamma p}^{\text{Cu}} < \lambda < \lambda_{\Gamma p}^{\text{Al}}$$

Это означает:
а) стенки медной сферы для этих нейтронов непроницаемы;
б) по алюминиевому нейтроноводу пойдут лишь те, что падают на стенку под углом больше критического

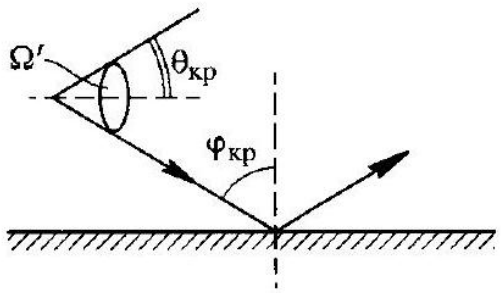


Рис. 180

$$\varphi_{\text{кр}} = \arcsin n = \arcsin \sqrt{1 - \frac{\lambda^2}{\left(\lambda_{\text{гр}}^{\text{A}}\right)^2}} = 42,1^\circ.$$

Поток нейтронов, падакщих на мишень, $\Phi = \langle j_\parallel \rangle S$, где $S = \pi r^2$ - площадь детектора, а $\langle i_\parallel \rangle$-тангенциальная по отношению к оси нейтроновода компонента плотности потока нейтронов, усредненная по телесному углу Ω (рис. 180), предельное значение которого

$$\Omega' = 2\pi\left(1 - \cos\theta_{\text{Кр}}\right) = 2\pi\left[1 - \cos\left(\frac{\pi}{2} - \varphi_{\text{Кр}}\right)\right].$$

Итак,

$$\langle j_\parallel \rangle = n_0 v \int \cos\theta \frac{d\Omega}{4\pi} = \frac{n_0 v}{4\pi} \int_0^{2\pi} d\varphi \int_0^{\pi/2-\varphi_{\text{кр}}} \cos\theta \sin\theta d\theta =$$
$$= \frac{n_0 v}{4} \sin^2\left(\frac{\pi}{2} - \varphi_{\text{Кр}}\right) = \frac{n_0 v}{4} \cos^2\varphi_{\text{Кр}}$$

Таким образом, искомый поток нейтронов на мишени

$$\Phi = S\frac{n_0 v}{4}\cos^2\varphi_{\text{К}p} = \frac{\pi r^2}{4} n_0 \sqrt{\frac{2\mathscr{E}}{m}} \cos^2\varphi_{\text{Кр}} \approx 18900 \text{ нейтронов /}.$$

8.

31. $\alpha = \frac{\lambda^2 |f| \rho N_{\text{A}} R}{2\pi A b} \approx 0,076$. Как видно из рис. 181 , по нейтроноводу пройдут лишь те нейтроны, которые падают на его поверхность под углом $\theta \leqslant \theta_{\text{кр}}$. Относительное их число α, очевидно, равно отношению h/b. Кроме того, приведем очевидные соотношения (i - угол падения):

$$\sin^2 i = \cos^2 \theta_{\text{Kp}} = n^2; 1 - \sin^2 \theta_{\text{K}p} = 1 - \frac{\lambda^2 N |f|}{\pi}.$$

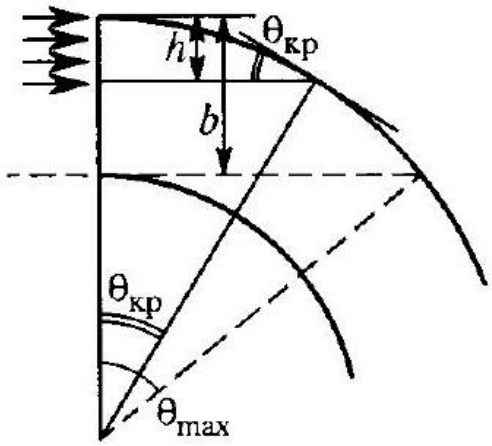


Рис. 181

8.

32. $R \approx \frac{4dm\&\lambda_0^2}{h^2 \theta_{\text{kp}}^2} \approx 75$ m.

8.

33. Отличие показателя преломления от 1 есть $1 - n = \frac{N_{\text{A}} \rho a \lambda^2}{2\pi A} = 4,74 \cdot 10^{-6}$. Тогда фокусное расстояние одного отверстия $F_1 = \frac{R}{2(1-n)} \approx \approx 10,5$ m, фокусное расстояние системы из 10 отверстий $F \approx 1$ м.

8.

40. $N_{\text{p}} = j_{\text{n}} \left[1 - \exp\left(-\frac{a}{\tau_{\text{n}} v}\right)\right] \approx 1,1 \cdot 10^6 \text{ см}^{-2} \cdot \text{с}^{-1}$, где $\tau_{\mathbf{n}} \approx 940$с - время жизни нейтрона.

8.

41: $\sigma = \frac{\eta A_{\text{Al}}}{\rho_{\text{B}} l_{\text{B}} N_{\text{A}}} \approx 0,04 \sigma$Н.
Решение. По определению сечения ядерной реакции

$$\sigma = \frac{dN/dt}{jN_{\text{M}}}$$

где dN/dt - число актов ядерного взаимодействия в единицу времени, [1/с]; j - плотность потока частиц, облучающих мишень $\left[1/\text{см}^2 \cdot \text{с}\right]$; $N_{\text{м}}$ - число ядер мишени.
Выход протонов определяется как

$$\eta = \frac{dN/dt}{jS}$$

где S - площадь поперечного сечения пучка. Тогда

$$\eta = \sigma \frac{N_{\text{M}}}{S} = \sigma n_{\text{M}} \qquad (*)$$

где $n_{\text{м}}$ $\left[1/\text{cm}^2\right]$ - поверхностная плотность ядер мешени.
Иногда эту же формулу записывают в несколько ином виде:

$$\frac{N}{S} = \sigma n_{\text{n}} n_{\text{M}},$$

где $n_{\text{п}}$ - число частиц пучка, приходящееся на 1 cm^2 сечения пучка, N число прореагировавших ядер мишени (число происшедших реакций).

Пробег α-частицы ограничен из-за потери энергии на ионизацию атомов. Очевидно, что потери пропорциональны плотности вещества, т. к. имеется приближенная пропорциональность между плотностью и порядковым номером Z элемента, а произведение пробега частицы l на эту плотность есть величина постоянная, практически не зависящая от рода вещества, а только от начальной энергии частицы. Таким образом,

$$l_{\text{B}} \rho_{\text{B}} = l_{\text{Al}} \rho_{\text{Al}}. \qquad (**)$$

Использую помеченные соотношения (*) и (**), получим

$$\sigma = \frac{\eta}{n_{\text{M}}} = \frac{\eta}{\frac{n_{\text{M}}}{l_{\text{Al}}} l_{\text{Al}}} = \frac{\eta}{n_{\text{Al}} l_{\text{Al}}},$$

где n_{Al} - концентрация ядер в алюминиевой мишени в $\left[\text{cm}^{-3}\right]$, l_{Al} - пробег α-частиц в ней. Однако в условии задан пробег $l_{\text{в}}$ - в воздухе. Подставляя $^{(**)}$ в выражение для σ, получим

$$\sigma = \frac{\eta \rho_{\text{Al}}}{n_{\text{Al}} \rho_{\text{B}} l_{\text{B}}} = \frac{\eta A_{\text{Al}}}{\rho_{\text{B}} l_{\text{B}} N_{\text{A}}} = 4 \cdot 10^{-26} \text{ cm}^2 = 0,04\sigma\text{H}.$$

Здесь использовано, что $\rho_{\text{Al}} = m_{\text{Al}} n_{\text{Al}}$, где m_{Al} - масса атома алюминия. Плотность воздуха при нормальных условиях подсчитывается по известной формуле для идеального газа

$$\rho_{\text{ВОЗ}} = \frac{P\mu}{RT} \approx 1,29 \cdot 10^{-3} \Gamma/\text{cm}^3.$$

8.

42. $\sigma(\mathcal{E}) = \frac{AC\mathscr{E}^2}{n_0}$.

8.

43. $\mathscr{J} = e\sqrt{\frac{KSc}{2l\varepsilon\sigma}} = 1,96$ А.

8.

44. $\frac{\Phi_2}{\Phi_1} = e^{-(\mu_2 - \mu_1)x}$. При $x = 5$ см $\frac{\Phi_2}{\Phi_1} \approx 1,5$.

8.

45. $\lambda' = 3\lambda = 3$Å.

18.2.5 Problems about neutrons 2

SOLUTIONS ABOUT NEUTRONS

8.

46. $\frac{N}{N_0} = \exp\left(-\frac{2P_0 N_\text{A}}{\mu g}\sigma\right) \approx 1,2 \cdot 10^{-6}$, где $\sigma = \pi r_N^2 = \pi r_0^2 A_N^{2/3}$ (это геометрическое сечение неупругого процесса поглощения, и поэтому дифракционную упругую добавку учитывать не нужно), P_0 - нормальное атмосферное давление, μ - молярная масса азота.

8.

47. $l_\text{p} = \frac{A_\text{H}}{8\pi\rho N_\text{A} r_\text{p}^2} \approx 148$ cm, $l_\text{N} = \frac{A_\text{H}}{2\pi\rho N_\text{A}(r_\text{N}+r_\text{p})^2} \approx 24$c. (См. также комментарий к ответу задачи 8.3 о дифракционном удвоении.)

8.48.

$\sigma_\text{погл} \simeq \frac{\pi}{2}\left(2R_\text{Pb} - R_\text{d}\right) R_\text{d} = 0,385$ бн.

8.

49. $T_\text{n} \approx \frac{\mathscr{E}_\gamma + \Delta\mathfrak{C}_\text{CB}}{1+M_\text{n}/M_\text{Li}} = 6,7$M В ; $T_\text{Li} = \mathscr{E}_\gamma + \Delta\mathscr{E}_\text{CB} - T_\text{n} = 1,1$M В, где $\Delta\mathscr{E}_\text{CB} = \mathscr{E}_2 - \mathscr{E}_1, M_\text{Li}$ - масса ядра ^{6}Li.

8.

50. $T_\text{p} = \frac{(4m_\text{p}-m_\pi)m_\pi}{2(m_\text{p}-m_\pi)}c^2 = 0,31$ ГэВ.

8.

51: $\varphi = \frac{\hbar_c}{\mathscr{E}_\gamma R_\text{d}} \approx 0,4$ рад.

Решение. Энергия связи нуклонов мала по сравнению с энергией падающих на мишень фотонов. Поэтому продольный импульс нуклонов можно оценить как $p_\parallel \approx \mathscr{E}_\gamma/$. Поперечный импульс нуклонов обусловлен движением нуклонов в ядре. Импульс нуклона в ядре оценим из соотношения неогг ределенностей

$$p_\perp \approx \Delta p \sim \frac{\hbar}{R_\text{d}} \approx 100\frac{\text{M В}}{c}, \quad c - \text{ скорость света.}$$

Таким образом, угол рассеяния нуклонов в пучке по порядку величины равен

$$\varphi \approx \frac{p_\perp}{p_\parallel} \approx 0,4 \text{ рад.}$$

8.

52. $p_{\text{O}^*} = m_{\text{O}^*}c\frac{\Delta\mathscr{E}}{2\mathscr{E}} = 1,49\frac{\text{Гэ В}}{c}, \alpha \approx \frac{p_{\text{O}^*}}{p} \approx 0,15$ рад.

8.

53. а) При реакции поглощается энергия (см. табл. 7 в конце книги)

$$Q = -931{,}5(7{,}016004 + 1{,}007825 - 7{,}016930 - 1{,}008665)\ \text{МэВ} = 1{,}645\ \text{МэВ}$$

б) Из закона сохранения энергии и импульса для неупругого процесса найдем, полагая $m_\text{n} = m_\text{p} = m_\text{Be}/7 = m_\text{Li}/7$:

1) в системе центра масс

$$\mathscr{E}_n^c = \mathscr{E}_\text{p}^\text{c} - \frac{7}{8}Q$$

2) в лабораторной системе

$$\mathscr{E}_\text{n} = \frac{49}{64}\left[\left(\mathscr{E}_\text{p} - \frac{8}{7}Q\right) + \frac{2}{7}\sqrt{\mathscr{E}_\text{p}\left(\mathscr{E}_\text{p} - \frac{8}{7}Q\right)}\cos\alpha_\text{c} + \frac{\mathscr{E}_\text{p}}{49}\right] =$$

$$= \frac{1}{64}\left[\sqrt{\mathscr{E}_\text{p}}\cos\alpha + \sqrt{49\left(\mathscr{E}_\text{p} - \frac{8}{7}Q\right) - \mathscr{E}_\text{p}\sin^2\alpha}\right]^2$$

где $\mathscr{E}_\text{n}^\text{c}$ и $\mathscr{E}_\text{n}$ - энергии нейтрона в системе центра масс и лабораторной системе, $\mathscr{E}_\text{p}^\text{c}, \mathscr{E}_\text{p}$ - то же для протона; α_c и α - углы между направлениями скорости протона и нейтрона в системе центра масс и лабораторной системе.

Из формул ясно, что минимальная энергия протона (порог реакции) в системе центра масс равна $\mathscr{E}_\text{p}^\text{c} = (7/8)Q = 1,44\text{М}$, а в лабораторной системе $\mathscr{E}_\text{p} = (8/7)Q = 1,88\text{М}$ эВ.

8.

54. $w \approx \frac{R\sigma\rho}{m_\text{N}} \approx 7 \cdot 10^{-6}$, где m_N - масса нуклона. Нейтрино взаимодействует только с нейтронами ядер.

8.

55. $\mathscr{E} \geqslant \frac{2m_\text{p}}{\rho R A} \approx 95 \cdot 10^3$ ГэВ.

8.

56. Ослабление потока нейтрино $\frac{\Delta\Phi}{\Phi} = \frac{\sigma N_\text{A}\rho 2R_3}{2A} = 4,2 \cdot 10^{-4}$.

8.

57*: Решение. Сечение взаимодействия нуклонов убывает с ростом скорости и стремится к «геометрическому» сечению $\sigma \sim 10^{-25}$ см^2 (радиус нуклона $r_\text{p} \approx 0,8 \cdot 10^{-13}$ см). Длина пробега при $n = 1$ см$^{-3}$

$$\lambda = \frac{1}{n\sigma} \approx 10^{25}\text{с} \approx 10^7 \text{ св. лет}$$

(1с. год $\approx 10^{18}$ см). Для массивных частиц в рамках геометрической модели рассеяния $\sigma \sim 10^{-24}$ см^2, а длина их свободного пробега $\lambda \sim 10^6$ св. лет. Т. о. прилет массивного «гостя» с такого расстояния крайне маловероятен. Заметим также, что полет комет по сильно выраженным гиперболическим траекториям не зафиксирован в истории астрономии.

8.

58. $M = \frac{\pi L^2 n\mu}{N_\text{A} N_\nu u\sigma t\eta} \approx 546$ т, где L - расстояние от Солнца до Земли, μ - молярная масса CCl_4.

8.

59: $\sigma \simeq 3 \cdot 10^{-46}$ cm^2.
Решение. Длина свободного пробега λ электрона в ядре, сечение взаимодействия σ и концентрация протонов n_p в ядре связаны известным соотношением $\lambda\sigma n_p = 1$. При этом $\lambda = 2v\tau$, где τ - время, проведенное K-электронами в ядре за $\tau_0 = 32$ дня, коэффициент «2» учитывает, что на K-оболочке находятся два электрона. Таким образом, искомое эффективное сечение

$$\sigma = \frac{1}{2nv\tau}$$

Концентрация протонов в ядре

$$n_{\text{p}} = \frac{Z}{\frac{4}{3}\pi r_0^3 A} = 5,3 \cdot 10^{37} \text{ cm}^{-3}$$

а время оценим как

$$\tau = \tau_0 \left(\frac{R_{\text{g}}}{r_1}\right)^3$$

где $R_{\text{я}} = 1,3 \cdot 10^{-13}$ A$^{1/3} = 4,3 \cdot 10^{-13}$ cm, а радиус орбиты K-электрона $r_1 = \frac{r_{\text{Б}}}{z-1} = 3,1 \cdot 10^{-10}$ cm. Таким образом, $\tau \approx 0,0074$c.
Оценку скорости K-электрона проведем, исходя из соотношения

$$\frac{mv^2}{2} = \text{Ry}(Z-1)^2$$

откуда

$$v = \sqrt{\frac{2\text{Ry}}{m}}(Z-1) = 3,7 \cdot 10^9 \frac{\text{cm}}{\text{c}}$$

Таким образом, искомое сечение

$$\sigma = \frac{1}{2nv\tau} \simeq 3 \cdot 10^{-46} \text{ cm}^2$$

8.

60. $R_{\mathbf{Pb}} = r_0 A^{1/3} \approx 7,7 \cdot 10^{-13}$ см. Для K-оболочки мюона в атоме Pb $r = r_{\text{E}} \frac{m_{\text{e}}}{m_\mu Z} \approx 3 \cdot 10^{-13}\text{c} < R_{\text{Pb}}$. Мюон взаимодействует с протоном по схеме $\mu^- + \text{p} \to \text{n} + \nu_\mu; \alpha \approx \frac{4\pi r_0^3 A}{3Z^2 \cdot c\tau\alpha} \approx 1,9 \cdot 10^{-41}$ cm^2, где $\alpha = \frac{e^2}{\hbar c} = \frac{1}{137}$.

8.

61*: Ослабление потока γ-квантов $j(L) = j(0)e^{-n_\sigma L}$ будет малым при условии $n\sigma L \ll 1$, где n - концентрация «поглотителей» - ядер ^{119}Sn, σ - сечение поглощения. Самопоглощение мессбауэровских квантов носит резонансный характер. Из формулы Брейта-Вигнера для сечения упругого процесса при $\mathscr{E}_\gamma = \mathscr{E}_{\text{рез}}$ получаем $\sigma = g\frac{4\pi}{k^2} = \frac{4\pi\hbar^2 c^2}{\mathscr{G}_\gamma^2}$. Здесь $g = \frac{1}{2} \cdot \frac{2J^*+1}{2J+1}$ - статистический фактор, учитывающий число начальных (возбужденное ядро с моментом J^*) и конечных (ядро в нормальном состоянии с моментом J плюс γ-квант) состояний. Здесь $2 = 2J + 1$ - число возможных проекций момента γ-кванта. Для ядра ^{119}Sn$J^* = 3/2, J = 1/2$ и $g = 1$. Кроме того, $n = \rho\frac{N_{\text{A}}}{\mu}\varepsilon f$. Отсюда $L \ll \frac{1}{n\sigma} = \frac{\mathscr{E}_\gamma^2 \mu}{4\pi\hbar^2 c^2 \rho N_{\text{A}} \varepsilon f} = 1,24 \cdot 10^{-3}$ см, где μ - молярная масса $BaSnO_3$.

8.

62. $N_{\text{Ar}} = \frac{jN_{\text{Cl}}\sigma}{\lambda}\left(1 - e^{-\lambda t}\right) \simeq 30$ ядер, где $N_{\text{Cl}} \approx 2,2 \cdot 10^{30}, \lambda = \frac{\ln 2}{T_{1/2}} \approx \approx 2,3 \cdot 10^{-7}\text{c}^{-1}$.

8.

63. $N_{\text{Ge}} \approx 5$ ядер.

8.

64. $\frac{\sigma_{\text{рез}}}{\sigma_0} \sim 10^6$. Здесь сечение поглощения в центре резонансной линии определяется формулой Брейта - Вигнера для неупругого поглощения $\sigma_{\text{рез}} = \pi\lambda^2 = \lambda^2/4\pi$.

8.

65. $\alpha_{\text{погл}} = \frac{j_0 - j_{\text{погл}}}{j_0} = 1 - e^{-n_{\text{м}}\,\sigma_{\text{погл}}\,d} \approx 0,1; \alpha_{\text{расс}} = \frac{j_0 - j_{\text{расс}}}{j_0} = 1 - e^{-n_{\text{м}}\sigma_{\text{расс}}d} \approx 0,37.$

8.

66. $\sigma_1 = \sigma_2 \frac{N_2^2 (kT)^2}{(2P_0)^2} \approx 11\sigma\text{Н}.$

8.

67. $a_{\text{эл}} = \frac{\pi\theta_{\text{кр}}^2 / \lambda^2 - N_2 a_2 + N_1 a_1}{z_2 N_2 - z_1 N_1} = -2,6 \cdot 10^{-16}$с. При учете рассеяния нейтронов на электронах, показатель преломления $n^2 = 1 - \frac{Na\lambda^2}{\pi} - \frac{ZNa_{\text{эл}}\,\lambda^2}{\pi}$. Кроме того, в данной задаче $\theta_{\text{кр}}^2 \approx n_1^2 - n_2^2$.

Возможны два различных механизма взаимодействия, приводящих к рассеянию нейтронов на электронах. Еще в 1947 г. Ферми указал на воз можность существования специфического взаимодействия между нейтроном и электроном, не сводящегося к взаимодействию между магнитными моментами этих частиц. Появление этого взаимодействия следует ожидать, исходя из представления о том, что ядерное взаимодействие есть результат обмена виртуальными пионами между нуклонами, так что часть времени нейтрон проводит в диссоциированном состоянии $n \rightleftarrows p + \pi^-$. Тем самым должны возникать силы притяжения, обусловленные электростатическим притяжением между электроном и протоном. Как следует из эксперимента, длина рассеяния очень мала и поэтому эти силы должны быть весьма короткодействующими. Нейтрон состоит из трех заряженных кварков, и это взаимодействие фактически есть взаимодействие между составляющими нейтрон кварками и электроном.

Второй механизм - это так называемое фолдиевское взаимодействие был получен и рассчитан Л. Фолди. Не вдаваясь в подробности, отметим, что взаимодействие медленного нейтрона с электростатическим полем возникает в результате учета квантовых эффектов и связано с «дрожанием» нейтрона в области размером в комптоновскую длину волны виртуальных пионов. На та ких расстояниях нейтрон уже нельзя считать точечной частицей.

8.

68. $\text{t} \approx \frac{m_{\text{n}} \mathring{\text{A}}_{\text{n}} \sigma_{\text{полн}}}{2h\Gamma_{\text{n}}} = 4,1 \cdot 10^{-15}$с.

8.

69: $\frac{\sigma_n(\mathscr{E}_1)}{\sigma_n(\mathscr{E}_2)} \approx 1$, т. е. сечения примерно равны.

Решение. Парциальное сечение нейтронного распада составного ядра

$$\sigma_{\text{n}} = \sigma_{\text{c}} \frac{\Gamma_{\text{n}}}{\Gamma_{\text{полн}}} = \sigma_{\text{c}} \frac{\Gamma_{\text{n}}}{\Gamma_{\text{n}} + \Gamma_{\text{y}}} \approx \sigma_{\text{c}} \frac{\Gamma_{\text{n}}}{\Gamma_{\text{y}}}$$

где сечение образования составного ядра $\sigma_{\text{c}} = \pi\hat{\hbar}^2 D$, а $D = 4\frac{kk'}{(k+k')^2} \approx \approx 4\frac{k}{k'} \propto \sqrt{\delta}$ - вероятность проникновения нейтрона в тяжелое ядро. Здесь $k = \frac{1}{\hbar}\sqrt{2m\mathscr{E}}; k' = \frac{1}{\hbar}\sqrt{2m\,(U_0 + \mathscr{E})} > k; \quad \hat{\lambda} = \frac{\hbar}{\sqrt{2m_{\mathscr{E}}}}$. Вероятность нейтрону покинуть составное ядро также пропорциональна D. Таким образом, $\sigma_n \propto \pi\lambda^2 D^2 \propto \frac{1}{\mathscr{E}}\mathscr{E} = \text{const}$, откуда и следует, что сечение распада составного ядра по нейтронному каналу от $\mathfrak{E}$ не зависит.

О3.1-8.19

Чему равна критическая скорость нейтронов, испытывающих полное отражение на границе вещества при произвольном угле падения? Число рассеивающих ядер в единице объема N и амплитуду рассеяния нейтронов f считать заданными.

О3.1-8.20

Найти критический угол скольжения чо для тепловых нейтронов с заданной длиной волны λ при отражении от материала с известными значениями N и f. При $\varphi < \varphi_0$ нейтроны полностью отражаются.

О3.1-8.21 Коэффициент преломления нейтронов

Вычислить коэффициент преломления нейтронов с энергией $\mathcal{E} = 2 \cdot 10^{-2}$ эВ в металлическом Be $\left(\rho \approx 1,85 \mathrm{g/cm^3}\right)$, если амплитуда рассеяния $f = -0,77 \cdot 10^{-12}$см. Чему равен угол полного отражения нейтронов?

О3.1-8.22

Максимальная скорость нейтронов, накапливаемых в ловушке в силу полного отражения от медных стенок, равна $v = 5,7$ m/c. Определить амплитуду рассеяния нейтронов на ядрах меди.

О3.1-8.23

После прохождения свинцовой пластинки толщиной $d = 2$ см интенсивность потока нейтронов с энергией $\mathcal{E} = 0,25$МВ уменьшилась и составила 70% от интенсивности падающего пучка. Показать, что это ослабление потока обусловлено преимущественно упругим изотропным s-рассеянием нейтронов ядрами свинца. Считая, что величина амплитуды рассеяния равна радиусу ядра, оценить размер ядра ^{208} Pb. Плотность свинца $\rho = 11,3 \mathrm{g/cm^3}$.

О3.1-8.24

Ультрахолодные нейтроны выходят широким пучком из горизонтального нейтроновода и затем движутся свободно над горизон тально расположенной пластинкой, упруго от нее отражаясь и тем самым совершая периодическое движение, как показано на рис. 49. Это движение в гравитационном поле квантуется, и поэтому пройдут над пластинкой только те нейтроны, у которых высота движения H соответствует разрешенной энергии. Оценить на основе правила квантования Бора-Зоммерфельда, какова третья разрешенная высота. См. задачу 3.6.

О3.1-8.25

Гравитационный рефрактометр (рис. 50) дает возможность оп ределить амплитуду рассеяния медленных нейтронов атомными ядрами, используя падение нейтронов в гравитационном поле Земли. Найти амплитуду рассеяния для ^{209}Bi, если известно, что для него на высоте $H = 60$ см резко изменяется скорость счета. Плотность висмута $\rho = 9,8 \mathrm{g/cm^3}$

О3.1-8.26

На рис. 51 показаны: реактор P, работающий на тепловых нейтронах, полая изогнутая труба (нейтроновод) и детектор нейтронов Д. Распределение нейтронов в реакторе по скоростям максвелловское при температуре $T \simeq 400$ K. Нейтроны, скорость v которых меньше граничной скорости ($v_p \sim 10$ m/c), называют ультрахолодными. Особенностью таких нейтронов является то, что они испытывают полное упругое отражение от стенок при любом угле падения. Найти зависимость скорости счета детектора от высоты колена H, полагая, что детектор одинаково эффективно регистрирует все ультрахолодные нейтроны. При каком значении H детектор не регистрирует ультрахолодные нейтроны?

О3.1-8.27

В реакторах, работающих на тепловых нейтронах, имеются очень медленные ультрахолодные нейтроны (УХН). Особенностью УХН является то, что при скоростях $v < v_{\text{гр}}$ (обычно граничная скорость $v \sim 10$ m/c) нейтроны упруго отражаются от стенок при любых углах падения. Для вывода УХН из реактора используют полые трубы - нейтроноводы. На рис. 52 изображен реактор P, нейтроновод специальной формы и на его конце - детектор нейтронов Д. Полагая, что распределение нейтронов по скоростям в реакторе максвелловское (при температуре $T \simeq 400$ K), найти, как зависит поток нейтронов, доходящих до детектора, от высоты его поднятия H. Оценить высоту $H_{\text{гр},}$, на которой поток нейтронов исчезает.

О3.1-8.28

В эвакуированном сосуде объемом $V = 1$ л находятся ультрахолодные нейтроны, отражающиеся от стенок с коэффициентом отражения, практически равным единице. В сосуде имеется отверстие площадью S, заклеенное фольгой, полностью прозрачной для ультрахолодных нейтронов. Какова должна быть площадь окошка 73 S, если наблюдаемое время хранения нейтронов в ловушке в 2 раза меньше среднего времени жизни свободных нейтронов $\tau \sim 10^3$ с. Считать, что скорость всех ультрахолодных нейтронов одинакова и равна $v = 5$ m/c.

О3.1-8.29

Вхождение нейтронов из вакуума в большинство веществ связано с преодолением энергетического барьера. Поэтому в замкнутой полости достаточно медленные нейтроны оказываются запертыми и могут накапливаться. Определить, какая доля из потока тепловых нейтронов, распределение по скоростям которых максвелловское, окажется запертой в медной камере. Предельный угол скольжения при полном «внешнем» отражении для нейтронов, движущихся со среднеквадратичной скоростью, составляет $i = 10$ угл. мин. Соударения нейтронов со стенками камеры могут рассматриваться как упругие.

О3.1-8.30

Монохроматические нейтроны с энергией $\mathscr{E} = 10^{-7}$ эВ транспортируются к мишени из источника (медной сферы радиусом R) по длинному круглому алюминиевому нейтроноводу радиусом $r = 10\text{см}R$. Концентрация нейтронов в источнике $n_0 = 1\text{с}^{-3}$ все время поддерживается постоянной, плотности алюминия и меди равны соответственно 2,7 и 8,9 г/см ^{3}, а их амплитуды когерентного рассеяния $-3,5 \cdot 10^{-13}$см и $-7,8 \cdot 10^{-13}$с. Вычислить поток нейтронов на мишени (распадом нейтронов пренебречь).
(пару пропустил)

18.2.6 Problems about neutrons 3

О3.1-8.34

Образец иода ^{127} I облучается нейтронным потоком такой интенсивности, что в 1 с образуется 10^7 атомов радиоактивного иода ^{128}I, период полураспада $T_{1/2}$ которого 25 мин. Найти число атомов ^{128} I и активность препарата через $1, 10, 25, 50$ мин после начала облучения. Каковы максимальные числа атомов ^{128} I и активность препарата при долгом облучении (т. е. при облучении до насыщения)?

8.

34: При облучении до насыщения число распадающихся в 1 с атомов йода (т. е. активность препарата) равно числу атомов, образующихся ежесекундно, т. е. $dn/dt = A = 10^7$ расп/с. Число атомов йода при активации до насыщения равно

$$N_{\text{нас}} = \frac{A}{\lambda} = 10^7 \frac{T}{\ln 2} = 2,16 \cdot 10^{10} \text{ атомов}$$

Число атомов йода через время t после облучения

$$N = N_{\text{нас}} \left(1 - e^{-\lambda t}\right)$$

или при малых $t (t \ll T)$

$$N = N_{\text{нас}}\, \lambda t = \dot{n} t$$

При $t = 1$ мин

$$N = At = 10^7 \cdot 60 = 6 \cdot 10^8 \text{ атомов.}$$

При $t = 25$ мин

$$N = N_{\text{нас}} \left(1 - e^{-\lambda t}\right) = 1,08 \cdot 10^{10} \text{ атомов}$$

О3.1-8.35

При облучении образца золота в потоке тепловых нейтронов плотностью $j = 10^{14}\text{см}^{-2} \cdot \text{с}^{-1}$ в реакторе в результате реакции $^{197}\text{Au}(\text{n}, \gamma)^{198}\text{Au}$ (сечение $\sigma_1 = 96$ бн) образуется β^--активный нуклид ^{198}Au, переходящий в ^{198}Hg с периодом полураспада $T_{1/2} = 2,7$ суток. В то же время, сечение реакции $^{198}\text{Au}(\text{n}, \gamma)^{199}\text{Au}$ очень велико и равно $\sigma_2 = 26000$ бн, так что изотоп ^{198} Au активно поглощает нейтроны (вторичная активация). На сколько уменьшается при учете вторичной реакции число образующихся ядер ^{198}Hg при времени облучения $t = 10T_{1/2}$?

8.

35: $\frac{N^*\left(10T_{1/2}\right)}{N\left(10T_{1/2}\right)} \approx \frac{\lambda}{\lambda+j\sigma_2} = 0,53.$

Решение. Пусть N_0 - исходное число ядер ^{197}Au, N^* - число ядер ^{198}Au. На изотопах золота идут следующие реакции:

$$\begin{array}{rcl} \mathrm{n} + {}^{197}\mathrm{Au} & \longrightarrow & {}^{198}\mathrm{Au} + \gamma \\ {}^{198}\mathrm{Au} & \xrightarrow{\beta^-} & {}^{198}\mathrm{Hg} \\ \mathrm{n} + {}^{198}\mathrm{Au} & \longrightarrow & {}^{199}\mathrm{Au} + \gamma. \end{array}$$

Уравнение баланса для ядер ^{198}Au имеет вид:

$$\frac{dN^*}{dt} \approx \sigma_1 j N_0 - \lambda N^* - \sigma_2 j N^* \qquad (*)$$

Обратим внимание на то, что в правой части в первом члене $\sigma_1 j N_0$ вместо текущего числа ядер ^{197}Au поставлено их исходное число N_0 (этим и обусловлен значок приближенного равенства). Простая оценка показывает, что за $t = 27$ суток ($t = 10T_{1/2}$) исчезнет всего

$$j\sigma_1 10T_{1/2} \approx 2 \cdot 10^{-3} = 0.2\% \quad \text{ядер} \quad {}^{197}\mathrm{Au}$$

что и обусловливает справедливость сделанного приближения.
Вычислим постоянную β^--распада ядер ^{198}Au

$$\lambda = \frac{\ln 2}{T_{1/2}} = 2,97 \cdot 10^{-6}\mathrm{c}^{-1}$$

а также второй коэффициент при N^* в уравнении (*)

$$\sigma_2 j = 2,6 \cdot 10^{-6}\mathrm{c}^{-1}$$

Решение дифференциального уравнения (*) имеет вид

$$N^*(t) = \frac{j\sigma_1 N_0}{\lambda + \sigma_2}\left\{1 - \exp\left[-\left(\lambda + j\sigma_2\right)t\right]\right\}$$

Вычислим показатель экспоненты

$$\left(\lambda + j\sigma_2\right) 10T_{1/2} \approx 13$$

Таким образом, $1 - e^{-13} \approx 1$. Отсюда следует, что

$$N^*(t) \approx \frac{j\sigma_{\mathrm{I}} N_0}{\lambda + j\sigma_2}.$$

Если бы за счет радиационного захвата нейтронов не «выгорали» ядра ^{198}Au, то

$$N(t) = \frac{j\sigma_1 N_0}{\lambda}\left(1 - e^{-\lambda t}\right) \approx \frac{j\sigma_1 N_0}{\lambda}.$$

Искомое уменьшение числа образующихся ядер ^{198}Hg равно

$$\frac{N^*\left(10T_{1/2}\right)}{N\left(10T_{1/2}\right)} \approx \frac{\lambda}{\lambda + j\sigma_2} = 0,53$$

О3.1-8.36

Образец золота ^{197}Au массой $m = 10$ мг облучали в потоке тепловых нейтронов плотностью $j = 10^{12}\mathrm{см}^{-2} \cdot \mathrm{с}^{-1}$ дважды: в течение первого дня с 9 до 17 час и в то же время на следующий день. Найти число образовавшихся радиоактивных ядер ^{198}Au $\left(T_{1/2} = 2,7\mathrm{су}\right.$, сечение активации, т. е. радиационного захвата нейтронов ядрами ^{197}Au, $\sigma = 96$ бн) к концу облучения во второй день. За какое время это же количество ядер ^{198}Au может быть получено при непрерывном облучении?

8.

36. $N = N_0\left(1 - e^{-\lambda t}\right)\left(1 + e^{-\lambda T}\right) = 1,4 \cdot 10^{14}$ ядер, где $T = 24$ ч; $t = 8$ ч (рис. 182). При непрерывном облучении $N = N_0\left(1 - e^{-\lambda t^*}\right)$, откуда $t^* = \frac{1}{\lambda}\ln\frac{N_0}{N_0 - N} = 14,5$.

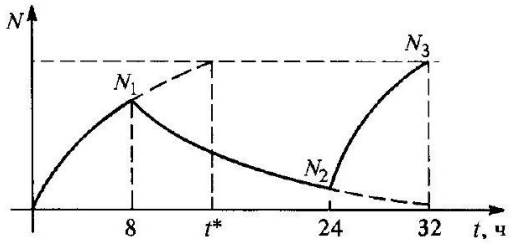


Рис. 182

О3.1-8.37

Образец алюминия облучается дейтронами с энергией 7МэВ, в результате чего происходит реакция $^{27}\mathrm{Al(d,p)}^{28}\mathrm{Al}$. Период полураспада ^{28}Al равен $T_{1/2} = 2,24$ мин. Облучение длится в течение $t_1 = 3,5$ мин, какое-то время t_2 уходит на перенос образца к детектору, а затем в течение времени $t_3 = 6$ мин производится измерение активности образца. Какую часть распадов регистрирует детектор от максимально возможного при том же времени переноса образца?

8.

37. $\frac{N_1}{N_1^{\max}} = \left(1 - e^{-\lambda t_1}\right)\left(1 - e^{-\lambda t_3}\right) = 0,55$, где $N_1^{\max} = n_0 e^{-\lambda t_2}$.

О3.1-8.38

Распространенность группы легких элементов Li, Be, B в Земле, Солнце, метеоритах намного меньше, чем более тяжелых C, N, O, однако в космических лучах содержание группы легких элементов Li, Be, B относительно группы c, N, O равно $\alpha = 0,34$. Это объясняется фрагментацией (развалом) C, N, O при прохождении через межзвездную среду, состоящую в основном из водорода. Оценить в г/см^2 количество водорода, которое должны при этом пройти высокоэнергетичные ядра C, N, O. Сечение деления (фрагментации) тяжелых элементов с образованием легких $\sigma_\phi = 90$ мбн, полное сечение их взаимодействия с водородом $\sigma_0 = 200$ мбн, фрагментацией легких элементов пренебречь.

8.

38. $l\rho = \frac{\ln(1+\alpha\sigma_0/\sigma_\phi)}{\sigma_0 N_\mathrm{A}} = 4,7\Gamma/\mathrm{cm}^2$.

О3.1-8.39

Сосуд объемом $V = 1$ л помещен в активную зону реактора на тепловых нейтронах с плотностью потока $j = 10^{12}\mathrm{см}^{-2} \cdot \mathrm{с}^{-1}$. Считая, что сосуд не возмущает пространственное максвелловское распределение нейтронов с $T = 300$ К, найти количество протонов, накопившееся в сосуде за счет распада нейтронов в течение $t = 6$ месяцев.

8.

39. За 6 месяцев накопится $1,08 \cdot 10^{14}$ протонов ($1,8 \cdot 10^{-10}$ г).

О3.1-8.44

При распаде ядра ^{60} Co одновременно (в каскаде) образуются два γ-кванта с энергиями $\mathscr{E}_1 = 1,17\mathrm{M} \ni \mathrm{B}$ и $\sigma_2 = 1,33$ МэВ соответственно. Определить, как изменится отношение потоков этих γ-квантов после их прохождения через свинец толщиной d и вычислить это отношение при $d = 5$ см. Коэффициенты ослабления потока γ-квантов в свинце равны соответственно $\mu_1 = 0,7\mathrm{см}^{-1}, \mu_2 = 0,62\mathrm{см}^{-1}$.

О3.1-8.45

При просвечивании детали монохроматическими тепловыми нейтронами с длиной волны $\lambda = 1$Å на изображении было обнаружено слабое темное пятно, свидетельствующее о наличии внутри детали инородного включения. Контраст изображения (отношение интенсивностей прошедших нейтронов в области включения к соседним однородным областям) был равен 1,26. Какова должна быть длина волны нейтрона, чтобы контраст возрос до 2? Считать, что сечение взаимодействия нейтронов с веществом носит нерезонансный характер.

МФТИ-ГКЭ.2020.5А Антинейтрино при бета-распаде

При β^--распаде ядра ^{137}Cs разность энергий покоя материнского и дочернего ядер ΔE составила две энергии покоя электрона. Электрон и антинейтрино разлетелись под углом $\alpha = 120°$. Дочернее ядро начало двигаться под углом $\varphi = 150°$ к направлению вылета электрона. Найти энергию вылетевшего антинейтрино в единицах энергии покоя электрона. Считать антинейтрино безмассовой частицей.

Первое Решение

Задача решается геометрией и релятивистской механикой (???)

Дочернее ядро движется в направлении, противоположном суммарному импульсу электрона и антинейтрино. Из равенства модулей составляющих их импульсов, перпендикулярных этому направлению, получаем $cp_e = ckp_v$, где $k^2 = \frac{\sin^2(\alpha+\varphi)}{\sin^2(\varphi)} = 4$. (?????)

Из закона сохранения энергии находим, вводя обозначения $x = \frac{\varepsilon_v}{m_e c^2}$, $\quad a = \frac{\Delta E}{m_e c^2} = 2$

$$a = x + \sqrt{1 + k^2 x^2}, \quad \text{откуда} \quad x = \frac{a - \sqrt{k^2\left(a^2-1\right)+1}}{1-k^2} = 0,54$$

Второе решение

(???)

Проектируя импульсы всех частиц на направление импульса электрона и перпендикулярное ему, получим

$$p_e = p_v \cos\left(180° - \alpha\right) + p_{\text{яд}} \cos\left(180° - \varphi\right)$$
$$p_v \sin\left(180° - \alpha\right) = p_{\text{яд}} \sin\left(180° - \varphi\right).$$

Из второго уравнения получаем $p_{\text{яд}} = \sqrt{3} p_v$, а из первого – $p_e = 2p_v$. Поскольку $\Delta E = 2m_e c^2 \ll M_{\text{яд}}\, c^2 (1\text{МВ} < 137$ ГэВ), то кинетической энергией ядра по сравнению с энергиями легких частиц можно пренебречь и закон сохранения энергии примет вид

$$\Delta E = p_v c + \sqrt{\left(p_e c\right)^2 + \left(m_e c^2\right)^2}$$

Подставляя сюда выражение для импульса электрона, получаем уравнение относительно $x = p_v c / \left(m_e c^2\right)$

$$\frac{\Delta E}{m_e c^2} = x + \sqrt{4x^2+1} \quad \text{или} \quad 2 - x = \sqrt{4x^2+1}$$

откуда

$$3x^2 + 4x - 3 = 0 \text{ и } x = \frac{\sqrt{13}-2}{3} \cong 0.54$$

P.S. Интересно, что при указанных в задаче углах, импульсы нейтрино и ядра оказываются взаимно перпендикулярными.

МФТИ-ГКЭ.2020.5А Электрон при бета-распаде

При β^--распаде ядра ^{137} Cs разность энергий покоя материнского и дочернего ядра ΔE составила две энергии покоя электрона. Дочернее ядро начало двигаться вдоль линии, являющейся биссектрисой угла разлёта электрона и антинейтрино. Найти кинетическую энергию вылетевшего электрона в единицах его энергии покоя. Массу антинейтрино считать равной нулю.

Первое решение.

Дочернее ядро движется в направлении, противоположном суммарному импульсу электрона и антинейтрино. Из равенства модулей составляющих их импульсов, перпендикулярных этому направлению, получаем $cp_e = ckp_v$, где $k^2 = 1$. Из закона сохранения энергии находим, вводя обозначения $x = \frac{\varepsilon_v}{m_e c^2}, a = \frac{\Delta E}{m_e c^2} = 2$: $a = x + \sqrt{1 + k^2 x^2}$, Откуда

$$x = \frac{a^2 - 1}{2a} = \frac{3}{4}; \frac{T_e}{m_e c^2} = a - x - 1 = 0,25.$$

Второе решение.

Проектируя импульсы всех частиц на направление импульса ядра и перпендикулярное ему, получим

$$p_{\text{яд}} = p_v \cos\alpha + p_e \cos\alpha$$
$$p_v \sin\alpha = p_{\text{яд}} \sin\alpha.$$

Из второго уравнения получаем $p_e = p_v$, а из первого $-- p_{\text{яд}} = 2p_v \cos\alpha$. Поскольку $\Delta E = 2m_e c^2 \ll M_{\text{яд}}\, c^2$(1МэВ $<<$ 137 ГэВ), то кинетической энергией ядра по сравнению с энергиями легких частиц можно пренебречь и закон сохранения энергии примет вид

$$\Delta E = p_v c + \sqrt{(p_e c)^2 + (m_e c^2)^2}$$

Подставляя сюда выражение для импульса электрона, получаем уравнение относительно $x = p_e c / \left(m_e c^2\right)$

$$\frac{\Delta E}{m_e c^2} = x + \sqrt{x^2 + 1} \text{ или } 2 - x = \sqrt{x^2 + 1}$$

откуда $x = 3/4$. Относительная кинетическая энергия электрона

$$\frac{T}{m_e c^2} = \sqrt{\left(\frac{p_e c}{m_e c^2}\right)^2 + 1} - 1 = \sqrt{x^2 + 1} - 1 = \frac{1}{4}$$

МФТИ-ГКЭ.2020.5В Антинейтрино при бета-распаде

При β^--распаде ядра ^{137}Cs разность энергий покоя материнского и дочернего ядра ΔE составила две энергии покоя электрона. Электрон и антинейтрино разлетелись под углом $\alpha = 90°$. Дочернее ядро начало двигаться под углом $\varphi = 150°$ к направлению вылета антинейтрино. Найти энергию вылетевшего антинейтрино в единицах энергии покоя электрона. Считать антинейтрино безмассовой частицей.

Решения

Решения просто дословно повторяю то же, что в предыдущих задачах, поэтому потом сам просто решу.

Дочернее ядро движется в направлении, противоположном суммарному импульсу электрона и антинейтрино. Из равенства модулей составляющих их импульсов, перпендикулярных этому направлению, получаем $cp_e = ckp_v$, где $k^2 = \frac{\sin^2(\varphi)}{\sin^2(\alpha+\varphi)} = \frac{1}{3}$. Из закона сохранения энергии находим, вводя обозначения
$x = \frac{\varepsilon_v}{m_e c^2}$, $a = \frac{\Delta E}{m_e c^2} = 2$

$$a = x + \sqrt{1 + k^2 x^2}, \quad \text{откуда } x = \frac{a - \sqrt{k^2\left(a^2 - 1\right) + 1}}{1 - k^2} = 0,88$$

О3.1-8.46

Оценить, какая доля ультрарелятивистких протонов космического излучения дойдет до поверхности Земли, не испытав ядерного взаимодействия.

О3.1-8.47

Оценить длины свободного пробега l_{p} и l_{N} ультрарелятивистских протонов и ядер азота в жидководородной камере. Радиус протона $r_p = 0,8 \cdot 10^{-13}$см, плотность жидкого водорода $\rho_{\text{H}} = 0,07\text{g/cm}^3$.

О3.1-8.48

Для создания пучков быстрых нейтронов часто используют взаимодействие релятивистских дейтронов с тяжелыми ядрами, когда в результате периферийного взаимодействия протон поглощается ядром - т.н. реакция срыва. Оценить сечение $\sigma_{\text{погл}}^{\text{такого процесса,}}$ когда мишенью служит абсолютно поглощающее нуклоны ядро свинца ^{208} Pb. Среднее расстояние между нуклонами в дейтроне равно $2R_{\text{d}} = 3,6$ фм.

О3.1-8.44

При распаде ядра ^{60} Co одновременно (в каскаде) образуются два γ-кванта с энергиями $\mathscr{E}_1 = 1,17\text{М} \ni \text{В}$ и $\sigma_2 = 1,33$ МэВ соответственно. Определить, как изменится отношение потоков этих γ-квантов после их прохождения через свинец толщиной d и вычислить это отношение при $d = 5$ см. Коэффициенты ослабления потока γ-квантов в свинце равны соответственно $\mu_1 = 0,7\text{см}^{-1}, \mu_2 = 0,62\text{см}^{-1}$.

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При просвечивании детали монохроматическими тепловыми нейтронами с длиной волны $\lambda = 1$Å на изображении было обнаружено слабое темное пятно, свидетельствующее о наличии внутри детали инородного включения. Контраст изображения (отношение интенсивностей прошедших нейтронов в области включения к соседним однородным областям) был равен 1,26. Какова должна быть длина волны нейтрона, чтобы контраст возрос до 2? Считать, что сечение взаимодействия нейтронов с веществом носит нерезонансный характер.

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(и там еще их много, не до других, итак кучу выгрузил.)

18.2.7 Problems about nuclear fission and reactors 1

О3.1-9.1

Кулоновские силы способствуют делению атомного ядра, а силы поверхностного натяжения препятствуют. Определить отношение кулоновской $\mathscr{E}_{\text{K}}$ и поверхностной $\mathscr{E}_{\text{п}}$ энергий атомного ядра, при котором деление на два равных осколка энергетически выгодно. Выразить то же условие через параметр деления Z^2/A, пользуясь формулой Вайцзеккера для энергий $\mathcal{O}_{\text{K}}$ и $\mathscr{E}_{\pi}$. Четности A и Z не учитывать.

9.

1*: Решение. При делении ядер на два равных осколка

$$\Delta\mathscr{E}_{\text{II}} = \mathscr{E}_{\text{I}}\left(2^{1/3} - 1\right), \Delta\mathscr{E}_{\text{кул}} = \mathscr{E}_{\text{кул}}\left(2^{-2/3} - 1\right)$$

где $\mathscr{E}_{\text{п}} = -17,8A^{2/3}$ [МэВ], $\mathscr{E}_{\text{кул}} = -0,71\frac{Z^2}{A^{1/3}}$ [МэВ].

Деление энергетически выгодно, когда $\Delta\mathscr{G}_{\text{п}} + \Delta\mathscr{E}_{\text{кул}} > 0$, т. е.

$$-|\mathscr{E}_{\text{II}}|\left(2^{1/3}-1\right)+|\mathscr{E}_{\text{ку}\Omega}|\left(1-2^{-2/3}\right)>0$$

Отсюда находим

$$\frac{\left|\text{Å}_{\text{кул}}\right|}{\left|\text{Å}_{\pi}\right|}>\frac{2^{1/3}-1}{1-2^{-2/3}}=0,70,\ \text{или}\ \frac{Z^2}{A}\geqslant 17,6.$$

О3.1-9.2

С помощью полуэмпирической формулы Вайцзеккера найти минимальное значение параметра Z^2/A, при котором становится энергетически возможным деление ядра с четным A и четным Z на две одинаковые части. Рассмотреть три случая: 1) $A/2$ - нечетное, $Z/2$ - произвольное; 2) $A/2$ - четное, $Z/2$ - нечетное; 3) $A/2$ четное, $Z/2$ - четное.

9.

2. 1) $\frac{Z^2}{A}\geqslant 17,62+129,4A^{-1,42}$; 2) $\frac{Z^2}{A}\geqslant 17,62+564,8A^{-1,42}$; 3) $\frac{Z^2}{A}\geqslant$
$\geqslant 17,62+305,9A^{-1,42}$.
Наметим путь решения задачи. Энергия связи четно-четного ядра

$$\mathscr{E}_{\text{СВ}}(A,Z)=\mathscr{E}_1A-\mathscr{E}_2A^{2/3}-\mathscr{E}_3\frac{Z^2}{A^{1/3}}-\mathscr{E}_4\frac{(A-2Z)^2}{A/2}-\mathscr{E}_5A^{-3/4}$$

где $\mathscr{E}_1=15,75;\mathscr{E}_2=17,8;\mathscr{E}_3=0,71;\mathscr{E}_4=23,7;\mathscr{E}_5=34$[М В]. Энергия связи половинок ядра

$$\mathscr{E}'_{\text{СВ}}\left(\frac{A}{2};\frac{Z}{2}\right)=\mathscr{E}_1\frac{A}{2}-\mathscr{E}_2\left(\frac{A}{2}\right)^{2/3}-\mathscr{E}_3\frac{(Z/2)}{(A/2)^{1/3}}-\mathscr{E}_4\frac{(A/2-Z)^2}{A/2}-\mathscr{E}_5\left(\frac{A}{2}\right)^{-3/4}\cdot\delta,$$

$$\text{где }\delta=\begin{cases}-1, & \text{если} \quad \frac{A}{2}=2p;\frac{Z}{2}=2k\\ 0, & \text{если} \quad \frac{A}{2}=2p+1,\\ +1, & \text{если} \quad \frac{A}{2}=2p;\frac{Z}{2}=2k+1.\end{cases}$$

Условие распада

$$2\mathscr{E}'_{\text{СВ}}\left(\frac{A}{2};\frac{Z}{2}\right)-\mathscr{E}_{\text{СВ}}\geqslant 0.$$

Далее легко получить приведенные выше ответы.

О3.1-9.3

Предполагая, что форма ядра является сферической, получить критерий устойчивости ядер по отношению к малым статическим деформациям формы. Ядерную материю считать несжимаемой. Проверить по полученному критерию устойчивость тяжелых естественных ядер. Как можно объяснить явления спонтанного деления?

У к а з а н и е. Площадь поверхности вытянутого эллипсоида вращения с полуосями a и b

$$S=2\pi ab\left(\frac{b}{a}+\frac{a}{\sqrt{a^2-b^2}}\arcsin\frac{\sqrt{a^2-b^2}}{a}\right)$$

Энергия равномерно заряженного по объему эллипсоида с зарядом Q равна

$$\mathcal{E}=\frac{3}{10}\frac{Q^2}{\sqrt{a^2-b^2}}\ln\frac{a+\sqrt{a^2-b^2}}{a-\sqrt{a^2-b^2}}.$$

9.

3* Решение. При деформации формы ядра изменяются энергия поверхностного натяжения и энергия кулоновского взаимодействия. Если $\Delta\mathfrak{E}_{\text{кул}}+\Delta\mathfrak{E}_{\text{пов}}\geqslant 0$, то энергия в конечном состоянии больше, и исходное сферическое ядро устойчиво:

$$\Delta\mathscr{E}_{\text{кул}}=\mathscr{E}^{\text{эллл}}_{\text{кул}}-\mathscr{E}^{\text{шар}}_{\text{Куал}};\quad \Delta\mathscr{E}_{\text{пов}}=\sigma\left(S^{\text{эллл}}-S^{\text{шар}}\right),$$

где σ - коэффициент поверхностного натяжения ядра. Будем статически "вытягивать» сферическое ядро радиусом r, превращая его в эллипсоид вращения с полуосями a и b. Введем эксцентриситет меридионального сечения

$$\varepsilon = \frac{\sqrt{a^2 - b^2}}{a}$$

Тогда $a = r\left(1-\varepsilon^2\right)^{-1/6}; ab = r^2\left(1-\varepsilon^2\right)^{1/6};$

$$\mathscr{E} = \frac{3}{5}\frac{Q^2}{r}\frac{\left(1-\varepsilon^2\right)^{1/3}}{2\varepsilon}\ln\frac{1+\varepsilon}{1-\varepsilon}$$

$$S = 4\pi r^2\frac{\left(1-\varepsilon^2\right)^{-1/6}}{2\varepsilon}\left(\sqrt{1-\varepsilon^2} + \frac{1}{\varepsilon}\arcsin\varepsilon\right)$$

При малых деформациях $\varepsilon \ll 0$. Эти выражения можно разложить в ряды и мы получаем:
Отсюда следует условие устойчивости ядра

$$\mathscr{E}_{\text{кул}}^{\text{шар}} / \mathscr{E}_{\text{П}} \leq 2.$$

Использовав формулу Вайцзеккера

$$\mathscr{E}_{\text{пов}} = 17,8A^{2/3}[\text{М В}] \text{ и } \mathscr{E}_{\text{кул}} = 0,71\frac{Z^2}{A^{1/3}}[\text{М В}]$$

легко получить искомый критерий устойчивости ядер к статическим деформациям формы

$$\frac{Z^2}{A} \leqslant 50$$

Рассмотренная задача - модельная, потому что большинство тяжелых ядер имеют несферическую форму.

Реально, конечно, процесс деления ядра - динамический. При взаимодействии нейтрона с ядром возникают колебания формы капли практически несжимаемой ядерной жидкости. Частота этих колебаний определяется соотношением $\mathscr{E}_{\text{кул}}$ и $\mathscr{E}_{\text{пов}}$. При $\mathscr{E}_{\text{кул}} / \mathscr{E}_{\text{пов}} \leqslant 2$ частота становится мнимой (колебания апериодическими), и амплитуда колебаний нарастает со временем. Это приводит к возникновению перетяжки, и ядро делится на два осколка.

О3.1-9.4

*: Оценить эффективное сечение деления ядра 235U нейтронами с энергиями 0,025 эВ (тепловые нейтроны) и 10 кэВ. Считать, что сечение деления равно сечению образования составного ядра. Ядерный потенциал аппроксимировать прямоугольной потенциальной ямой глубиной 40МВ.

9.

4: $\sigma = \frac{4\pi}{kk'} \approx \begin{cases} 2600 & \text{бн (тепловые нейтроны)}, \\ 4,16\text{Н}(\mathscr{E} = 10 \text{ кэВ}), \end{cases}$

где $k = \frac{1}{\hbar}\sqrt{2m\mathscr{E}}, k' = \frac{1}{\hbar}\sqrt{2m\left(\mathcal{E}+U_0\right)}$.

Решение. При энергиях тепловых нейтронов дебройлевская длина волны нейтрона $\lambda = \hbar/\sqrt{2m\mathscr{E}} = 3\cdot 10^{-9}$ cm $> R_{\text{U}} = 8\cdot 10^{-13}$ cm и сечение образования составного ядра $\sigma \approx \pi\hbar^2 D$, где D - коэффициент прохождения нейтронной волной границы ядра. Коэффициент прохождения D определяется соотношением (см. задачу 3.25)

$$D = \frac{4kk'}{\left(k+k'\right)^2} \approx \frac{4k}{k'}$$

где волновые числа k и k' определяются как коэффициенты в уравнениях Шредингера для областей вне ядра и внутри ядра (рис. 183)

$$k = \frac{1}{\hbar}\sqrt{2m\mathscr{E}}, k' = \frac{1}{\hbar}\sqrt{2m\left(\mathscr{E}+U_0\right)}.$$

Искомое сечение взаимодействия

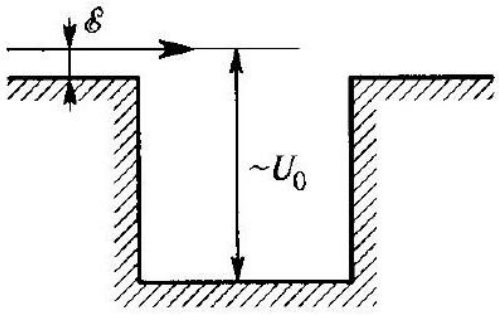


Рис. 183

$$\alpha \approx \frac{4\pi}{kk} \approx \frac{2\pi\hbar^2}{m\sqrt{\varrho}U_0} \approx 2600\sigma\text{Н}$$

Для нейтрона с энсргией 10 кэВ $\hat{t} \approx 3 \cdot 10^{-9}$ см, и искомое сечение $\sigma \approx 4,16$Н. Как видно из формулы, при данных энергиях $\sigma \propto 1/\sqrt{\S} \propto 1/v$. Такая зависимость сечения деления от скорости нейтронов называстся законом Бете. Здесь он имеет место, поскольку рассматриваемые энергии лежат далеко от области резонансного поглощения нейтронов ядрами ^{235}U$(1 \div 100$ э В).

О3.1-9.5

Сечение деления ^{238}U быстрыми нейтронами с энергией $= 5$МВ равно $\sigma(n,f) = 0,5$ бн. Какова относительная вероятность этого нерезонансного процесса по отношению ко всем процессам, идущим через компаунд-состояние? Глубину потенциальной ямы ядра урана принять равной $U = 50$ МэВ.

9.

5. $\sigma_\text{с} = \pi(R+\lambda)^2 D = 2,3\sigma$Н, где $D = \frac{4k_1k_2}{(k_1+k_2)^2} \approx 0,7$. Относительная вероятность деления к полной вероятности реакций, идущих через составное ядро, $\frac{\Gamma_\text{дел}}{\Gamma_\text{сост}} = \frac{\sigma_\text{дел}}{\sigma_\text{с}} \simeq 0,2$.

О3.1-9.6

Размножение нейтронов в делящейся среде можно условно представить как смену поколений. Существовавшие в некоторое время нейтроны будут все рано или поздно поглощены ядрами. На смену «умершему» поколению нейтронов появится новое поколение нейтронов, которое опять через некоторое время «умрет», чтобы дать «жизнь» следующему поколению. Конечно, время жизни нейтронов неодинаково, но можно ввести среднее время жизни одного поколения, точно так же, как это делается для человеческих поколений. Отношение числа нейтронов второго поколения к числу нейтронов первого поколения в делящейся среде называется коэффициентом размножения k_∞. Если $k_\infty < 1$, то говорят, что система находится в подкритическом состоянии. Число нейтронов в такой системе будет уменьшаться во времени. Пусть в подкрити ческой бесконечной системе в некоторый момент времени появилось N_0 нейтронов. Определить общее число нейтронов, образующихся в системе, если исходное их число равнялось N_0.

9.

6. $N = \frac{N_0}{1-k_\infty}$.

О3.1-9.7

Показать, что в системе из чистого ^{238}U нельзя достигнуть $k_\infty > 1$ (см. задачу 9.6). Для энергии нейтронов больше 1,1 МэВ се- чение поглощения не превышает величины 10^{-24}см^2 : $\sigma_\text{погл} = \sigma_\text{дел} + \sigma_\text{захв} < 10^{-24}$см^2, где $\sigma_\text{дел}$ - сечение деления, а $\sigma_\text{захв}$ - сечение радиационного захвата. В то же время сечение упругого рассеяния, при котором нейтрон теряет относительно большую часть своей энергии, $\sigma_\text{расс} \simeq 3 \cdot 10^{-24}$см^2.

9.

7. $k_\infty = \frac{\sigma_{\text{расс}}}{\sigma_{\text{погл}}} \frac{\sigma_{\text{дел}}}{\sigma_{\text{погл}} + \sigma_{\text{расс}}}$. В данном случае $k_\infty = 0,75 < 1$, что и требовалось показать.

О3.1-9.8 характерное время T реактора (??)

Реактивностью реактора называют величину $\rho = \frac{k-1}{k}$, где k - коэффициент размножения нейтронов; если $|k-1| \ll 1$, то $\rho \approx k-1$. Найти в этом приближении изменение мощности $W(t)$ реактора в надкритическом режиме, когда $k > 1$. Определить характерное время T реактора, т.е. время возрастания мощности W в e раз. Среднее время жизни одного поколения нейтронов равно т.

9.

8. $P(t) = P(0)k^{t/\tau} \approx P(0)e^{t \ln k/\tau} \approx P(0)e^{\rho t/\tau}; T = \frac{\tau}{\rho}$.

О3.1-9.9

При каких значениях реактивности реактора ρ, определенного в предыдущей задаче, запаздывающие нейтроны определяют зависимость мощности от времени? Доля запаздывающих нейтронов $\beta = 0,0064$.

9.9.

При $\rho < \beta$. В отсутствие запаздывающих нейтронов $k - \beta < 1$ реакция только на мгновенных делительных нейтронах затухла бы. При $\rho > \beta$ реакция может развиваться и без запаздывающих нейтронов.

О3.1-9.10

Активная зона ядерного реактора заполнена смесью урана и графита, имеющей при бесконечных размерах коэффициент размножения нейтронов $k_\infty = 1,05$. Среднее расстояние, проходимое нейтроном от места рождения до поглощения, $L = 50$ см. Оценить критический радиус реактора R, при котором полное число нейтронов остается постоянным, считая, что плотность нейтронов изменяется линейно по радиусу и равна нулю на границе.

О3.1-9.11

В работающем ядерном реакторе в числе многих элементов из урана все время образуются изотопы иода ^{135} I, претерпевающие следующую последовательность бета-распадов (периоды полураспада указаны)

$^{135}\text{I} \overset{6.744\text{ac}}{\rightarrow} {}^{135}\text{Xe} \overset{9.24\text{qac}}{\longrightarrow} {}^{135}\text{Cs} \rightarrow \ldots$

Так как ядра ^{135} Xe обладают очень большим сечением поглощения нейтронов, в работающем реакторе накопления этого изотопа не происходит. Однако при остановке реактора ксенон начинает накапливаться, тем самым уменьшается коэффициент размножения нейтронов и сразу же повторный запуск реактора затрудняется (образуется так называемая иодная яма). Через какое время после остановки реактора количество ядер ^{135} Xe будет максимальным? Считать, что в момент остановки реактора ядер ксенона в нем нет.

О3.1-9.12

Один из способов утилизации оружейного плутония (почти чистый ^{239}Pu) состоит в его облучении в реакторе, где за счет захвата (поглощения) нейтронов ^{239}Pu либо делится, либо переводится в ^{240}Pu, который в свою очередь переходит в ^{241}Pu. Сечения этих реакций равны $\sigma_{f1} = 741, \sigma_{n1} = 267, \sigma_{n2} = 290$ бн. Плутоний считается непригодным для создания ядерного оружия, если содержание в нем ^{240}Pu составляет 40% от ^{239}Pu. Определить время, необходимое аля достижения этой концентрации ^{240}Pu в образце оружейного плутония в реакторе с массой $M = 2,75$ т ^{235}U и мощностью $W = 3500$МВ. Сечение деления ^{235}U равно $\sigma_{f3} = 579$ бн, в одном акте деления выделяется энергия $\varepsilon = 180\text{M} \ni \text{В}$.

МФТИ-ГКЭ.2021.5 Полураспад (!!!!!!)

Сечение деления урана- 238γ-квантами с энергией $E_0 = 3$ МэВ составляет $\sigma = 0,1$ нбн. Если плотность потока энергии в пучке γ-квантов превышает $S = 740$ мкВт / см^2, то в куске урана массой $m = 10$ г за время $t_0 = 10$ ч можно заметить вклад вынужденного деления на фоне спонтанного. Оценить по этим данным период полураспада $T_{1/2}$ урана-238.

Solution

(???)

Радиоактивный распад в результате спонтанного деления описывается уравнением $\frac{dN_{\text{сп}}}{dt} = \lambda N$, где $\lambda = \frac{\ln 2}{T_{1/2}}, N = N_{\text{A}}\frac{m}{A} = 2,53 \cdot 10^{22}$. Поскольку $t_0 \ll T_{1/2}$, то среднее число распавшихся атомов равно $N_{\text{сп}} = \lambda N t_0$. Так как радиоактивный распад является случайным процессом, то возможны отклонения от среднего числа порядка $\delta N_{\text{сп}} = \sqrt{\lambda N t_0}$. Распад в результате вынужденного деления описывается уравнением $\frac{dN_{\text{вын}}}{dt} = \sigma \Phi N$, где Φ - плотность потока квантов. Процесс вынужденного деления можно заметить, если число таких распадов за время наблюдения превысит отклонение от среднего в спонтанном процессе распада: $N_{\text{вын}}\ (t_0) = \sigma \Phi N t_0 \geq \delta N_{\text{сп}} = \sqrt{\lambda N t_0}$, откуда $\Phi \geq \frac{1}{\sigma}\sqrt{\frac{\lambda}{N t_0}}$. Считая поток γ-квантов монохроматическим, находим $\Phi = S/E_0$. Из этих двух соотношений, получаем $T_{1/2} \geq \left(\frac{E_0}{S\sigma}\right)^2 \frac{\ln 2}{N t_0} \cong 3,19 \cdot 10^{22}\text{с} \approx 10^{15}$ лет.

О3.1-9.13

Под действием нейтронной компоненты космического излучения на поверхности Земли из ^{238}U образуется ^{239}Pu. Считая, что плотность потока космических нейтронов равна $j_{\text{n}} = 1\ \text{м}^{-2} \cdot \text{с}^{-2}$ и эффективное сечение захвата (поглощения) нейтронов ядром урана равно $\sigma = 3$ бн, определить отношение концентрации ^{239}Pu и ^{238}U при временах $t \gg T_{1/2}$ от начала облучения $\left(T_{1/2} = 2,4 \cdot 10^4\right.$ лет - период полураспада плутония).

О3.1-9.14

Много лет тому назад в урановом месторождении в Окло (Габон, Африка) «работал» природный ядерный реактор на ^{235}U. Из $_3$ массы $M = 200$ т имевшегося там урана выделилась энергия $\mathscr{E} = 10^{11}\text{В}^-$. Оценить, какая часть массы $^{235}\text{U}\Delta M/M$ была при этом израсходована, если его начальная концентрация составляла $n_0 = 3,5\%$ Время «работы» реактора много меньше периода полураспада урана. Энергию $\mathscr{E}_0$, выделяющуюся при делении ядра ^{235}U, принять равной 200МВ

О3.1-9.15

Естественный уран состоит из $99,3\%$ изотопа ^{238}U и $0,7\%$ 235U. При обогащении смеси изотопов ^{235}U до 3% возможна цепная реакция деления. Какое время t тому назад такой природный реактор мог «загореться»?

О3.1-9.16

В урановом реакторе мощностью $W = 1$ МВт образуется в среднем $N = 6$ антинейтрино на один акт деления ядра урана. Энергия антинейтрино & $= 1,5$ МэВ. Реактор окружен биологической защитой (бетон). Оценить плотность потока антинейтрино j за биологической защитой на расстоянии $L = 5$ м и долю энергии э, уносимой антинейтрино из реактора. Считать, что реактор имеет сферическую форму.

О3.1-9.17

При спонтанном делении тяжелых элементов (тория, урана) внутри Земли выделяется мощность $W \simeq$ 15 ТВт. Делящиеся элементы являются источниками антинейтрино (≈ 6 антинейтрино на акт распада). Предполагая распределение элементов в Земле равномерным, оценить плотность потока антинейтрино на ее поверхности. Сечение поглощения антинейтрино принять равным $\sigma = 10^{-43}\text{см}^2/$ нуклон.

О3.1-9.18

Во всем мире в 1978 г. была выработана тепловая энергия, эквивалентная сжиганию около 10^{10} т условного топлива. Условное топливо имеет тепловыделение 7000 кал на 1 г. Какое количество естественного урана потребовалось бы взамен сжигания 10^{10} т условного топлива для получения такого же

количества тепловой энергии? Считать, что в реакторах коэффициент воспроизводства «ядерного горюго» к числу атомов затраченного). За один акт деления выделяется 200 МэВ энергии. В естественном уране содержится $0,714\%235\mathrm{U}$.

О3.1-9.19

Один из перспективных методов получения новых изотопов - синтез сверхтяжелых ядер с их последующим распадом. Найти пороговую скорость v ядер урана, бомбардирующих урановую мишень, для реакции

$$^{238}_{92}\mathrm{U} + ^{238}_{92}\mathrm{U} \to ^{476}_{184}\mathrm{X} \to \sum \mathrm{X}_i$$

18.2.8 Problems about nuclear fission and reactors 2

О3.1-9.20

В термоядерном реакторе концентрация дейтерия $n_\mathrm{d} = 2,5 \cdot 10^{15}$ ядер/см cm^3 поддерживается на постоянном уровне с помощью внешнего источника дейтронов, который обеспечивает поступление q ядер/(с cm^3). Принимая во внимание только реакции (d,d) и (d,t), найти: 1) установившуюся концентрацию n_t трития $\mathrm{t}; 2)$ вели- 84 чину $q; 3)$ мощность W, выделяемую в 1 см ^{3} плазмы. При температуре плазмы $T = 60$ кэВ усредненные по максвелловскому распределению произведения сечений реакций на относительную скорость частиц равны $\overline{\sigma v_\mathrm{dd}} = 1,6 \cdot 10^{-17}\mathrm{см}^3 \cdot \mathrm{c}^{-1}; \overline{\sigma v_\mathrm{dt}} = 10^{-15}\mathrm{см}^3 \cdot \mathrm{c}^{-1}$.

О3.1-9.21

Каково количество термоядерных реакций, происходящих в $1\mathrm{см}^3$ в 1с, если известно сечение реакции $\sigma(v)$, где v-относительная скорость реагирующих дейтронов, а n - число дейтронов в $1\mathrm{см}^3$?

О3.1-9.22

Какая плотность тепловой мощности $W\left[/c \cdot \mathrm{cm}^3\right]$ со- ется термоядерными реакциями в чисто дейтериевой плазме с концетрацией ядер $n_\mathrm{d} = 10^{15}\mathrm{см}^{-3}, \overline{\sigma v_\mathrm{dd}} = 10^{-17}\mathrm{см}^3/\mathrm{c}$, что соответствует температуре плазмы $4,6 \cdot 10^8$ К или 40 кэВ в энергетических единиах? При вычислениях vчитывать лишь энергию реакиий $\mathrm{d} + \mathrm{d}$.

9. Деление ядер. Реакторы. Термоядерный синтез

9.

10: $R = \sqrt{\frac{3}{k_\infty - 1}} L = 4$ m.

Решение. Полное число нейтронов

$$N = \int_0^R n_0 \left(1 - \frac{r}{R}\right) 4\pi r^2 dr = \frac{\pi n_0 R^3}{3}$$

где n_0 - концентрация нейтронов при $r = 0$. Полагая $L \ll R$, подставляя числовые данные получим, что из тонкого наружного слоя реактора, содержащего $4\pi R^2 L \frac{n_0 L}{2R}$ нейтронов (где $\frac{n_0 L}{2R}$ - средняя плотность нейтронов внутри этого слоя), примерно половина этих нейтронов уйдет из реактора, а половина останется. За это же время внутри реактора появится $(k_\infty - 1) N$ новых нейтронов. Таким образом,

$$\pi R n_0 L^2 = \frac{1}{3} \pi n_0 R^3 (k_\infty - 1)$$

откуда и следует ответ $R = \sqrt{\frac{3}{k_\infty - 1}} L = 400$ см.

9.

11*** $t^* = \frac{T_1 T_2 \ln(T_2/T_1)}{(T_2 - T_1)\ln 2} \approx 11$ час.

Решение. Пусть при $t = 0$ имсется N_0 ядер йода I, а ядер ксенона Xe $N_2(0) = 0$. Процесс β-распада / описывается уравнением

$$dN_1 = -N_1 \lambda_1 dt$$

откуда $N_1(t) = N_0 e^{-\lambda_1 t}$, где λ_1 - постоянная распада ядер йода. Ядра ксенона не только постоянно образуются из йода, но и одновременно распадаются с постоянной распада λ_2. Запишем уравнение этого процесса и его решение:

$$dN_2 = -N_2\lambda_2 dt + N_1\lambda_1 dt$$
$$N_2(t) = ae^{-\lambda_1 t} + be^{-\lambda_2 t}$$

Поскольку $N_2(0) = 0$, то $a = -b, N_2(t) = b\left(e^{-\lambda_2 t} - e^{-\lambda_1 t}\right)$. Подстановка $N_1(t)$ в дифференциальное уравнение для N_2 дает

$$b(\lambda_1 - \lambda_2) = N_0\lambda_1, \text{ откуда } b = \frac{N_0\lambda_1}{\lambda_1 - \lambda_2}$$

Таким образом,

$$N_2(t) = \frac{\lambda_1 N_0}{\lambda_1 - \lambda_2}\left(e^{-\lambda_1 t} - e^{-\lambda_2 t}\right)$$

Условие максимума числа ядер ксенона $\frac{dN_2}{dt} = 0$, откуда $\ln\frac{\lambda_1}{\lambda_2} = (\lambda_1 - \lambda_2)\,t^*$. Таким образом, искомое время

$$t^* = \frac{T_1 T_2 \ln(T_2/T_1)}{(T_2 - T_1)\ln 2} \approx 11 \text{ час.}$$

9.

12* $t = 3,4 \cdot 10^7$с ≈ 390 дней.

Решение. Полное нейтронное сечение σ_t ^{239}Pu складывается из сечеиия деления σ_{f1} и сечения радиационного захвата нейтрона σ_{n1} (переход в ^{240}Pu), т. е. $\sigma_t = \sigma_{f1} + \sigma_{\text{nl}} = 1008\sigma$Н.

Пусть плотность потока нейтронов, облучающих ^{239}Pu, равна $j\left[\text{ см}^{-2}\cdot\text{с}^{-1}\right]$. Тогда число ядер N_1 ^{239}Pu убывает по закону

$$\frac{dN_1}{dt} = -j\sigma_t N_1$$

У равнение, описывающие накопление ядер N_2 ^{240}Pu с учетом их распада имеет вид:

$$\frac{dN_2}{dt} = j\sigma_{n1}N_1 - j\sigma_{\text{n2}}N_2.$$

Решение этой системы уравнений (см. задачу 9.11) есть

$$N_1 = N_{10}\exp(-j\sigma_t t)\,; N_2 = \frac{\sigma_{\text{n1}}N_{10}}{\sigma_{\text{n2}} - \sigma_t}\left[\exp(-j\sigma_t t) - \exp(-j\sigma_{\text{n2}}t)\right]$$

Требуемое отношение концентраций

$$\frac{N_{240}}{N_{239}} = 0,4 = \frac{N_2}{N_1} = \frac{\sigma_{\text{n1}}}{\sigma_{\mathbf{n2}} - \sigma_t}\left\{1 - \exp\left[-j\left(\sigma_{\text{n2}} - \sigma_t\right)t\right]\right\}$$

откуда

$$-j\left(\sigma_{\text{n2}} - \sigma_t\right)t = \ln\left(1 - 0,4\frac{\sigma_{\text{n2}} - \sigma_t}{\sigma_{\text{n1}}}\right).$$

Плотность потока j находится из энергетических соображений. Мощность реактора W равна (N_3 - число ядер горючего)

$$W = \varepsilon j\sigma_{j3}N_3 = \varepsilon j\sigma_{f3}MN_{\text{A}}/235$$

откуда искомый поток нейтронов

$$j = \frac{235W}{\varepsilon\sigma_{f3}MN_{\text{A}}} \approx 3\cdot 10^{13}\text{ см}^{-2}\cdot\text{с}^{-1}$$

Время наработки необходимой концентрации ^{240}Pu равно

$$t = \frac{\ln\left[1 + 0,4\left(\sigma_t - \sigma_{\text{n2}}\right)/\sigma_{\text{n1}}\right]}{j\left(\sigma_t - \sigma_{\text{n2}}\right)} = 3,4\cdot 10^7\text{с} \approx 390 \text{ дней.}$$

9.

13. $\frac{n_{\mathrm{Pu}}}{n_{\mathrm{U}}} = \frac{\sigma j_{\mathrm{n}} T_{1/2}}{\ln 2} \approx 3,3 \cdot 10^{-16}$.

9.

14. $\frac{\Delta M}{M} = \frac{\mathscr{E}_{\mathrm{U}} m_{\mathrm{n}}}{\mathscr{C}_0 M n_0} \approx 0,63$, где $A_{\mathrm{U}} = 235$.

9.

15. $t = \frac{T_1 T_2}{(T_1 - T_2)\ln 2} \ln\left(\frac{N_{10}}{N_{20}} \frac{N_2}{N_1}\right) \approx 1,7 \cdot 10^9$ лет, где $T_1 = 4,5 \cdot 10^9$ лет, $T_2 = 0,7 \cdot 10^9$ лет - периоды полураспада ^{238}U и ^{235}U.

9.

16. $j = \frac{WN}{4\pi L^2 Q} \approx 6 \cdot 10^{10}$ см$^{-2} \cdot$ с$^{-1}$; $\eta = \frac{N}{Q} = 0,045$, где $Q = 200$М В энергия, выделяемая при делении ядра урана.

9.

17* Земля практически не поглощает антинейтрино, поэтому $j = \frac{6W}{Q 4\pi R_3^2} \approx 6 \cdot 10^5$ см$^{-2} \cdot$ с$^{-1}$.

Решение. В соответствии с законами сохранения электрического и лептонного зарядов антинейтрино взаимодействуют только с протонами:

$$\tilde{\nu}_{\mathrm{e}} + \mathrm{p} \to \mathrm{n} + \mathrm{e}^+$$

Реакция взаимодействия $\tilde{\nu}_{\mathrm{e}}$ с нейтронами невозможна в силу закона сохранения лептонного заряда. Наибольшее поглощение толщей Земли будут испытывать антинейтрино, проходящие внутри Земли максимальный путь, равный диаметру Земли. Концентрация нуклонов $n = \rho/m_{\mathbf{H}} = \rho N_{\mathrm{A}}/\mu_{\mathrm{H}}$, где m_{H} - масса нуклона; $\mu_{\mathrm{H}} = 1$ г/моль. Поскольку Земля состоит в основном из элементов с $A \leq 60$, то числа протонов и нейтронов примерно равны, т. е. $n_p = n/2$. Тогда число протонов в «столбике» длиной $2R_3$ с поперечным сечением 1 см^2

$$N_{\mathrm{p}} = n_{\mathrm{p}} 2R_3 = \frac{1}{2}\frac{\rho N_{\mathrm{A}}}{\mu_{\mathrm{H}}} 2R_3 = \frac{\rho N_{\mathrm{A}} R_3}{\mu_{\mathrm{H}}}$$

Уравнение, описывающее убыль антинейтрино из потока,

$$dN_v = -\sigma N_v dN_{\mathrm{p}}$$

Интегрируя это уравнение, получим

$$N_v = N_0 e^{-\sigma N_{\mathrm{p}}} = N_0 \exp\left\{-\sigma \frac{\rho N_{\mathrm{A}} R_3}{\mu_{\mathrm{H}}}\right\},$$

где N_0 - начальный поток антинейтрино. Поскольку показатель экспоненты

$$\frac{\sigma \rho N_{\mathrm{A}} R_3}{\mu_{\mathrm{H}}} \approx 1,4 \cdot 10^{-10} \ll 1,$$

то $N_v \approx N_0$, т. е. Земля практически не ослабляет поток антинейтрино, т. е. поглощением антинейтрино Землей можно пренебречь.

Полный поток антинейтрино на поверхности Земли от распада распре деленных по объему ядер тяжелых элементов равен потоку от всех распадающихся ядер, помещенных в центре Земли. По существу это аналог электростатической теоремы Гаусса. Поэтому

$$j = \frac{6W/Q}{4\pi R_3^2} = 6 \cdot 10^5 \frac{\text{нейтрино}}{\text{см}^2 \cdot \text{с}},$$

где $\boldsymbol{W} = 15$ ТВ - мощность, выделяемая подземными источниками деления, $Q = 200$М Э - энергия, выделяющаяся при одном акте деления.

9.

18. $m = 282,6 \cdot 10^3$ т естественного урана.

9.19.

$v = \frac{\sqrt{2}Ze}{\sqrt{MR_{\text{g}}}} \approx 3,5 \cdot 10^9$ см /с, где Z, M, R_{g} - порядковый номер, масса и радиус ядра урана.

9.

20: 1) $n_{\text{t}} = 10^{13}$ см$^{-3}$; 2) $q = 1,25 \cdot 10^{14}$с$^{-1} \cdot$ см$^{-3}$; 3) $W = 99,6$ВТ/см^3.
Решение. Отметим энерговыделение при указанных реакциях синтеза ядер

$$\text{d} + \text{d} \to \begin{cases} \text{t} + \text{p}, & Q_1 = 3,94\text{M В}; \\ {}^3\text{He} + \text{n}, & Q_2 = 3,26\text{M В}; \end{cases}$$
$$\text{d} + \text{t} \to {}^4\text{He} + \text{n}, \quad Q_3 = 17,6\text{M} \ni \text{В}.$$

Первые две реакции (d, d) идут с равной вероятностью в силу зеркаль ности ядер t и ^{3}He. Изменение со временем концентрации частиц в резуль тате взаимодействия определяется скоростями реакций (d, d) и (d, t) и скоростью поступления ядер извне.

Скорость реакции - это число столкновений частиц сорта 1 и 2 в единицу времени, приводящее к реакции. Пусть $f_1(\mathbf{v}_1)$ и $f_2(\mathbf{v}_2)$ - функции распределения частиц сортов 1 и 2 по скоростям. Будем считать, что эти функции нормированы, т. е. $\int f(\mathbf{v}) d\mathbf{v} = 1$. Тогда каждую секунду в каждом см ^{3} объема плазмы число актов взаимодействия частиц, имеющих скорости от v_1 до $v_1 + dv_1$, и от v_2 до $v_2 + dv_2$ равно

$$dN_{12} = n_1 f_1(\mathbf{v}_1)\, n_2 f_2(\mathbf{v}_2)\, |\mathbf{v}_1 - \mathbf{v}_2|\, \sigma(|\mathbf{v}_1 - \mathbf{v}_2|)\, d\mathbf{v}_1 d\mathbf{v}_2,$$

где n_1 и n_2 - плотности частиц, $\sigma(v)$ - сечение реакции, зависящее от относительной скорости частиц, $\mathbf{v} = \mathbf{v}_1 - \mathbf{v}_2$ (рис. 184). Следовательно,

$$N_{12} = \iint d\mathbf{v}_1 d\mathbf{v}_2 n_1 f_1(\mathbf{v}_1)\, n_2 f_2(\mathbf{v}_2)\, v\sigma(v) \quad \left[\text{см}^{-3} \cdot \text{с}^{-1}\right]$$

Считая, что пнотность частиц n_1 и n_2 неизменны, получаем

$$N_{12} = n_1 n_2 \overline{\sigma v}, \quad \text{где} \quad \overline{\sigma v} = \iint d\mathbf{v}_1 d\mathbf{v}_2 f_1(\mathbf{v}_1)\, f_2(\mathbf{v}_2)\, v\sigma(v').$$

Запишем уравнение для изменения концентрации ядер дейтерия n_{d} со временем

$$\frac{\partial n_{\text{d}}}{\partial t} = -2\frac{(n_{\text{d}} - 1)\, n_{\text{d}}}{2}\overline{\sigma v_{\text{dd}}} - n_{\text{d}} n_{\text{t}} \overline{\sigma v_{\text{dt}}} + q.$$

Здесь первое слагаемое описывает убыль ядер дейтерия из-за столкновений друг с другом. Одно ядро d имеет $(n_{\text{d}} - 1)$ столкновений (в расчете на единицу объема); n_{d} ядер имеют $n_{\text{d}}(n_{\text{d}} - 1) \approx n_{\text{d}}^2$

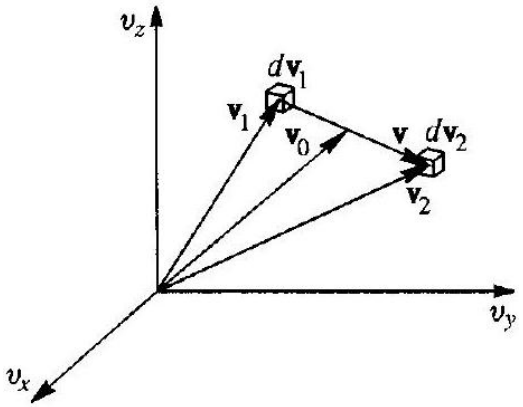


Рис. 184 столкновений. Для реакции (d, d) безразличен порядок дейтронов в паре, поэтому число взаимодействующих пар равно $n_{\text{d}}^2/2$, и в каждом акте реакции исчезают два дейтрона. Таким образом,

$$\frac{\partial n_{\text{d}}}{\partial t} = -n_{\text{d}}^2 \overline{\sigma v_{\text{dd}}} - n_{\text{d}} n_{\text{t}} \overline{\sigma v_{\text{dt}}} + q.$$

Аналогично, для ядер трития можно записать:
$\frac{\partial n_\mathrm{t}}{\partial t} = -n_\mathrm{t} n_\mathrm{d} \overline{\sigma v_\mathrm{dt}} + \frac{1}{2}\frac{n_\mathrm{d}(n_\mathrm{d}-1)}{2}\overline{\sigma v_\mathrm{dd}}$.
Во втором слагаемом первый коэффициент 1/2 учитывает вероятность получения трития в результате столкновения пары дейтронов. Таким образом,

$$\frac{\partial n_\mathrm{t}}{\partial t} = -n_\mathrm{t} n_\mathrm{d} \overline{\sigma v_\mathrm{dt}} + \frac{1}{4} n_\mathrm{d}^{2\overline{\sigma v}}\mathrm{dd}.$$

В стационарном состоянии производные $\dot{n}_\mathrm{d}$ и $\dot{n}_\mathrm{t}$ равны нулю, и мы получаем уравнения баланса

$$\begin{cases} q = n_\mathrm{d}^2 \overline{\sigma v_\mathrm{dd}} + n_\mathrm{d} n_\mathrm{t} \overline{\sigma v_\mathrm{dt}}, \\ \frac{1}{4} n_\mathrm{d}^2 \overline{\sigma v_\mathrm{dd}} = n_\mathrm{d} n_\mathrm{t} \overline{\sigma v_\mathrm{dt}}, \end{cases}$$

откуда вычисляем стационарную концентрацию ядер трития

$$n_\mathrm{t} = \frac{1}{4} n_\mathrm{d} \frac{\langle \sigma v_\mathrm{dd} \rangle}{\langle \sigma v_\mathrm{dt} \rangle} = 10^{13}\ \mathrm{cm}^{-3},$$

а также интенсивность поступления в зону реакции дейтронов от внешнего источника

$$q = \frac{5}{4} n_\mathrm{d}^2 \overline{v v_\mathrm{dd}} = 1,25 \cdot 10^{14} \frac{\text{ядер}}{\mathrm{c} \cdot\ \mathrm{cm}^3}.$$

Выделяющаяся в термоядерных реакциях мощность W может быть выражена через скорости изменения концентраций ядер дейтерия по каналам (d, d) и (d, t)

$$W = Q_\mathrm{dd} \frac{1}{2} \left(\frac{\partial n_\mathrm{d}}{\partial t} \right)_\mathrm{dd} + Q_\mathrm{dt} \left(\frac{\partial n_\mathrm{d}}{\partial t} \right)_\mathrm{dt},$$

где Q_dd и Q_dt - энерговыделения в реакциях (d, d) и (d, t). Коэффициент 1/2 учитывает, что для реакции (d, d) нужно два дейтрона. Поскольку эта реакция идет с равной вероятностью по двум каналам, то $Q_{dd} = \frac{Q_1+Q_2}{2}, Q_\mathrm{dt} = Q_3$. Окончательно,

$$\boldsymbol{w} = n_\mathrm{d}^2 \overline{\sigma v_\mathrm{dd}} \frac{Q_1 + Q_2 + Q_3}{4} = 9,96 \cdot 10^8 \frac{9\mathrm{pr}}{\mathrm{ccm}^3} = 99,6 \frac{\mathrm{Br}}{\mathrm{cm}^3}.$$

9.

21. Число реакций, происходящих в 1 с в 1 cm^3, равно $n^2 \overline{\sigma(v)v}/2$, где черта означает усреднение по всем значениям относительных скоростей атомов дейтерия (см. задачу 9.20).

9.

22. $W = \frac{n_\mathrm{d}^2}{2} \overline{\alpha v_\mathrm{dd}} \left(\frac{3,94+3,26}{2} \right) = 2,88 \cdot 10^7 \frac{\text{Дж}}{\mathrm{c} \cdot \mathrm{cm}^3} = 2,88 \frac{\mathrm{Вт}}{\mathrm{cm}^3}$ (см. также задачу 9.20).

9.

27. $R > \frac{12 \sigma_\mathrm{c} T^4}{Q \eta_\mathrm{d}^2 \sigma v_\mathrm{dd}} = 3,45 \cdot 10^{10}\ \mathrm{cm} = 3,45 \cdot 10^5 \mathrm{KM}$,
$Q = Q_1 + Q_2 + Q_3 = 24,8\mathrm{MB}$ - выделение энергии, соответствующие суммарному уравнению синтеза $5\ \mathrm{d} \to {}^3\mathrm{He} + {}^4\mathrm{He} + \mathrm{p} + 2\mathrm{n}, \sigma_\mathrm{c}$ - константа Сте-фана-Больцмана.

9.

28: $\frac{N_\mathrm{dd}^{\mathrm{KB}}}{N_\mathrm{dd}^{\mathrm{KJ}}} \approx 1,6 \cdot 10^{21}$.
Решение. Как следует из решения задачи 9.20, скорость реакции (d, d) можно представить в виде

$$N_\mathrm{dd} = \frac{n_\mathrm{d}^2}{2} \overline{\sigma v_\mathrm{dd}}, \quad \text{где } \overline{\sigma v_\mathrm{dd}} = A(m,T) \int_0^\infty v^3 \exp\left(-\frac{\mu v^2}{2kT} \right) \sigma(v) dv,$$

где $\mu = m/2$ - приведенная масса, v - относительная скорость.
При классическом рассмотрении реакция произойдет только тогда, когда кинетическая энергия относительного движения будет больше высоты кулоновского барьера $\mu v^2/2 \geqslant U_{\text{кул}} = e^2/(2R_\mathrm{d})$, где R_d

- классический радиус дейтрона ($R_{\text{d}} = 1,7 \cdot 10^{-13}$ cm). В этом случае сечение взаимодействия $\sigma_{\text{KI}}(v) = 4\pi R_{\text{d}}^2$ и

$$\overline{\sigma v}_{\text{dd}}^{\text{KJ}} = A\int_0^\infty v^3\sigma_{\text{K}\Omega}(v)\exp\left(-\frac{\mu v^2}{2kT_0}\right)dv = \tilde{A}\pi\left(\frac{e^2}{U_{\text{ky}}}\right)^2\int_{U_{\text{ky}}}^\infty \mathscr{E}\exp\left(-\frac{\mathscr{E}}{kT_0}\right)d\mathscr{E} \approx$$
$$\approx \tilde{A}\pi\left(\frac{e^2}{U_{\text{y}\boldsymbol{J}}}\right)^2(kT_0)^2\left(\frac{U_{\text{Ky}}}{kT_0}+1\right)\exp\left(-\frac{U_{\text{Ky}}}{kT_0}\right) \approx$$
$$\approx \tilde{A}\pi\left(\frac{e^2}{U_{\text{ky}}}\right)^2 kT_0U_{\text{ky}}\exp\left(-\frac{U_{\text{Ky}}}{kT_0}\right)$$

поскольку $\frac{U_{\text{кул}}}{kT_0} \approx 58 \gg 1$.

При вычислениях были введены обозначения $\mathscr{E} = \mu v^2/2, \tilde{A} = A(2/\mu)^2$.

В квантовом случае определяющую роль играет проницаемость кулоновского барьера. При $\mathscr{E} \ll U_{\text{кул}}$ (это условие выполняется в задаче, поскольку $\mathscr{E} \sim (3/2)kT \approx 1,4 \cdot 10^4$ эВ $\ll 0,5$М Э)

$$D(\mathscr{E}) \simeq \exp\left(-\frac{4e^2}{\hbar}\sqrt{\frac{2\mu}{\mathscr{E}}}\right)$$

В этом случае сечение взаимодействия $\sigma_{\text{кв}}(\mathscr{E}) = \sigma(\mathscr{E})D(\mathscr{E})$, где $\sigma(\mathscr{E})$ геометрическое сечение образования составного ядра, и

$$\overline{\sigma v}_{\text{dd}}^{\text{KB}} = A\int_0^\infty v^3\sigma_{\text{KB}}(v)\exp\left(-\frac{\mu v^2}{2kT_0}\right)dv = \tilde{A}\int_0^\infty \mathscr{E}\sigma_{\text{KB}}(\mathscr{E})\exp\left(-\frac{\mathscr{E}}{kT_0}\right)d\mathscr{E};$$
$$\sigma_{\text{KB}}(\mathscr{E}) = \sigma(\mathscr{E})D(\mathscr{E}) \approx \sigma(\mathscr{E})\exp\left(-\frac{4e^2}{\hbar}\sqrt{\frac{2\mu}{\mathscr{E}}}\right)$$

Выражение для $\overline{\sigma v}_{dd}^{\text{KB}}$ содержит интеграл с произведением двух экспонент (падающей и медленно растущей). Главную роль здесь играет область значений энергий вблизи максимума показателя экспоненциальной функции

$$\frac{d}{d\mathscr{E}}\left(\frac{\mathscr{E}}{kT_0}+\frac{4e^2\sqrt{2\mu}}{\hbar\sqrt{\mathscr{E}}}\right)\Big|_{\mathscr{E}=\mathscr{E}_{\max}} = 0$$

откуда

$$\S_{\max} = 2kT_0\sqrt[3]{\frac{\mu e^4}{\hbar^2 kT_0}} = 3,1 \cdot 10^4 \ni \text{ В}$$

Соответствующая длина волны де Бройля $\hat{\lambda} = \frac{\hbar}{\sqrt{2\mu\varphi_{\max}}} = 3,66 \cdot 10^{-11}\text{c} \gg R_{\text{d}}$. Таким образом, в наиболее существенной области значений энергий справедлива аппроксимация $\sigma(\mathscr{E}) = \pi\hbar^2 = \pi\hbar^2/(2\mu)$ и

$$\bar{\sigma}_{\text{d d}}^{\text{KB}} = \tilde{A}\frac{\pi\hbar^2}{2\mu}\int_0^\infty \exp\left(-\frac{\mathscr{E}}{kT_0}-\frac{4e^2}{\hbar}\sqrt{\frac{2\mu}{\mathscr{G}}}\right)d\mathscr{E}$$

Подынтегральное выражение представляет собой функцию с острым максимумом и шириной порядка kT_0. Т.к. $kT_0 > \mathscr{E}_{\max}$, то спадание функции вблизи экстремума определяется экспонентой $\exp(-\mathscr{E}/kT_0)$. Таким образом,

$$\overline{\sigma v}_{\text{dd}}^{\text{KB}} = \tilde{A}\frac{\pi\hbar^2}{2\mu}kT_0\exp\left(-\frac{\mathscr{E}_{\max}}{kT_0}-\frac{4e^2\sqrt{2\mu}}{\hbar\sqrt{\mathscr{E}_{\max}}}\right) = \tilde{A}\frac{\pi\hbar^2}{2\mu}kT_0\exp\left(-6\sqrt[3]{\frac{\mu e^4}{\hbar^2 kT_0}}\right)$$

Окончательно,

$$\frac{N_{\text{dd}}^{\text{KB}}}{N_{\text{dd}}^{\text{KJ}}} = \frac{\hbar^2}{2\mu e^4}U_{\kappa\text{y}}\exp\left(\frac{U_{\text{Ky}}}{kT_0}-6\sqrt[3]{\frac{\mu e^4}{\hbar^2 kT_0}}\right) \approx 1,6 \cdot 10^{21}$$

9.

29: В магнитном поле все столкновения идут с моментом импульса $J = 3/2$ и среднее сечение увеличивается в 1,5 раза.

Решение. При низких энергиях, т. е. при малых импульсах, дебройлевская длина волны очень велика по сравнению с размерами частиц. По правилу квантования момента импульса взаимодействие возможно только в состоянии с $\mathbf{L} = 0$, и полный момент импульса ядра как целого - чисто спиновый. Полный момент импульса системы $d + t : I = \mathbf{S}_d + \mathbf{S}_\mathrm{t}$ может принимать два значения $I = 3/2$ и $I = 1/2$. Так как ядерные силы зависят от спинов сталкивающихся частиц и полный спин есть интеграл движения, то

$$\langle\sigma\rangle = w_{3/2}\sigma_{3/2} + w_{1/2}\sigma_{1/2}$$

Здесь $\langle\sigma\rangle$ - среднее сечение реакции; $\sigma_{3/2}$ и $\sigma_{1/2}$ - сечения реакции, соответствующие $I = 3/2$ и $I = 1/2; w_{3/2}$ и $w_{1/2}$ - доли состояний, соответствующие значениям полного момента импульса I из общего числа состояний, равного $(2S_\mathrm{d} + 1)(2S_\mathrm{t} + 1)$. По условию $\sigma_{1/2} \approx 0$, тогда $\langle\sigma\rangle = w_{3/2}\sigma_{1/2} = \frac{2\cdot(3/2)+1}{(2\cdot1+1)(2\cdot1/2+1)}\sigma_{3/2} = \frac{2}{3}\sigma_{3/2}$. В магнитном поле, полностью поляризующем спины взаимодействующих ядер, возможно только одно состояние $S_{\mathrm{d}z} = 1$ и $S_{\mathrm{t}z} = 1/2; J_z = 3/2$ (ось z совпадает с направлением магнитного поля B). Тогда $\langle\sigma(B)\rangle = \sigma_{3/2}$ и, следовательно, среднее сечение возрастает в 1,5 раза.

9.

30: Если учесть четыре реакции

$$\mathrm{d} + \mathrm{d} \to \mathrm{t} + \mathrm{p} + 3{,}94\ \text{М эВ};$$
$$\mathrm{d} + \mathrm{d} \to {}^3\mathrm{He} + \mathrm{n} + 3{,}26\text{М} \ni \ \text{В};$$
$$d + {}^3\mathrm{He} \to \alpha + \mathrm{p} + 18{,}3\text{М эВ};$$
$$\mathrm{d} + \mathrm{t} \to \alpha + \mathrm{n} + 17{,}6\text{М} \to \ \text{В},$$

то на один "сгоревший» дейтрон выделяется энергия 7,18 МэВ. Пользуясь этим, легко найти, что при полном сгорании дейтерия, содержащегося в 1 л воды, выделится энергия $3{,}6 \cdot 10^3\text{КВ} \cdot$, что равно энергии, получающейся ири сгорании 277 кг бензина.

9.

31. $\mathscr{E} = 3 \cdot 10^7$ кДж.

9.

32. $\frac{\mathscr{E}_{\text{кин}}}{\text{конечн}} = \frac{36kT}{3Q_1+2Q_2+2Q_3} \approx 0{,}06,$

где Q_1, Q_2, Q_3 - энергии, выделяющиеся при реакциях синтеза, равные соответственно 3,3; 4; 17, 6М ЭВ.

9.

33. $n_\mathrm{d}\tau = \frac{3kT}{\frac{\eta}{\eta-1}\overline{\sigma v_\mathrm{dd}}\frac{2Q_\mathrm{dd}+Q_\mathrm{dt}}{4} - 1{,}5\cdot10^{-34}\sqrt{T}} \approx 7 \cdot 10^{15}\mathrm{c/cm}^3.$

Решение. Реакция будет самоподдерживающейся, если выделяемая в реакторе плотность мощности превысит плотность мощности совокупных

потерь: $W \geqslant W_\text{пот}$. Последняя состоит из тепловых потерь, связанных с уходом частиц из зоны реакции, и потерь на тормозное излучение:

$$\boldsymbol{W} = \boldsymbol{W}_\mathrm{T} + \boldsymbol{W}_\text{изЗл}$$

Выделяемая в реакторе мощность W берется из мощности термоядерного синтеза W_0 и частичного полезного преобразования мощности потерь в корпусе реактора, так и в окружающей защите

$$\boldsymbol{W} = \eta\boldsymbol{W}_0 + \beta\left(\boldsymbol{W}_\mathrm{T} + \boldsymbol{W}_\text{из3.}\ \right)$$

Таким образом, условие стационарной работы на уровне нулевой мощности при $\eta = \beta$

$$\eta \cdot (W_0 + W_{\text{Т}} + W_{\text{изл}}) = W_{\text{Т}} + W_{\text{изл}}$$

Используя выражения для $\boldsymbol{W}_0$ и $W_{\text{Т}}$, полученные в задачах 9.20 и 9.24 ,

$$W_0 = n_{\text{d}}^2 \overline{\sigma v}_{\text{dd}} \frac{1}{4} (2Q_{\text{dd}} + Q_{\text{dt}}), W_{\text{Т}} = \frac{3 n_{\text{d}} kT}{\tau}$$

получим

$$n_{\text{d}}\tau = \frac{3kT}{\frac{\eta}{\eta-1}\overline{\sigma v}_{\text{dd}}\frac{2Q_{\text{dd}}+Q_{\text{dt}}}{4} - 1,5 \cdot 10^{-34}\sqrt{T}} \approx 7 \cdot 10^{15} \text{c/см}^3$$

9.

34. $\eta = \frac{Q}{Q_{\text{П}}} = \frac{4{,}964}{24{,}68} = 0,2.$

9.

35. $\mathscr{E}_{\text{K}}^{\max} = 19,8\text{М ВВ}.$

9.

36. $= \frac{e m_{\text{p}}}{\sigma l t} \approx 9300$ А.

9.

37: $t_{1/2} = 1,2 \cdot 10^{10}$ лет - время, за которое концентрация протонов убывает в два раза.

Решение. Согласно решению задачи 9.20 уравнение, описывающее изменение концентрации протонов, имеет вид

$$\frac{dn_{\text{p}}(t)}{dt} = -\frac{n_{\text{p}}^2(t)}{2}\overline{\sigma v_{\text{p}}} \approx -\frac{n_{\text{p}}^2(t)}{2}\sigma\bar{v}$$

где $n_{\text{p}}(0) = \rho N_{\text{A}} = 9,25 \cdot 10^{25}$ см$^{-3}$ начальная плотность ядер водорода, $\bar{v} = \sqrt{\frac{8kT}{\pi m_{\text{p}}}} = 5,6 \cdot 10^7$ см/с - средняя тепловая скорость протонов. Интегрируя это уравнение, получаем

$$\frac{1}{n_{\text{p}}(t)} - \frac{1}{n_{\text{p}}(0)} = \frac{\sigma\bar{v}t}{2}.$$

Откуда следует, что концентрация протонов уменьшается вдвое за время $t_{1/2} = \frac{2}{n_{\text{p}}(0)\sigma\bar{v}} = 1,2 \cdot 10^{10}$ лет.

9.

38. Эффект можно заметить, если число ядер, подверженных вынужденному делению, $N_{\text{вын}}$ превысит дисперсию фона, т. е. дисперсию числа спонтанно делящихся ядер $N_{\text{сп}}$. Дисперсия фона $\sqrt{\overline{\Delta N_{\text{c}}^2}} \approx \sqrt{N_{\text{c}}'} = \sqrt{\lambda N t_0}$.

За время t_0 $\overline{N_{\text{вын}}} \approx \sigma N j t_0$, где N - число ядер урана в момент времени t. Таким образом, $j \geqslant \frac{1}{\sigma}\sqrt{\frac{A \ln 2}{T_{1/2} N_{\text{A}} m t_0}} \approx 5 \cdot 10^{10}$ см$^{-2} \cdot$ с$^{-1}$.

9.39.

Грубая оценка: $R \sim \lambda \approx \frac{1}{n\sigma} = \frac{A}{\rho N_{\text{A}} \sigma} \approx 4,2$ см, откуда масса «шарика» $M \approx 5,7$ кг. Более точный рассчет дает $R \approx \frac{3A}{\sigma\rho N_{\text{A}}(\upsilon-1)} \approx 8,3$ см и $M \approx 45$ кг.

9.

40. $t = \frac{n}{n_0\sigma\sqrt{2\S/M}} \simeq 2\cdot 10^{-4}$с, где n_0 - концентрация ядер ^{235}U, M - масса нейтрона, n - число поколений нейтронов, сменившихся к моменту заданного выделения энергии деления: n находится из уравнения $\frac{k_\infty^n-1}{k_\infty-1} = \frac{W}{\mathscr{E}_{\text{дел}}}$, где $\mathscr{E}_{\text{дел}} \simeq 200$М В/акт деления, $n \approx 3,27\cdot 10^4$.

9.

41* $\beta = \left(\frac{\hbar c}{E_\gamma r_0 A^{1/3}}\right)^2 \approx 17$.

Решение. Фотоделение через состояние I^-происходит при поглощении $E1$ (электрических дипольных) квантов, а через состояние 2^+- при поглощении $E2$ (квадрупольных) квантов. Так как энергия гамма-квантов болыше высоты барьеров, то отношение вероятностей деления определяется только отношением сечений поглощения квантов ядром, равным $\beta = (\lambda/R_{\text{я}})^2$. Здесь $\hat{\lambda} = \lambda/2\pi$ - приведенная длина волны γ-кванта, а $R_{\text{я}}$ радиус ядра. Таким образом, отношение равно

$$\beta = \left(\frac{\hbar c}{E_\gamma r_0 A^{1/3}}\right)^2 \simeq 17$$

Это значит, что происходит преимущественное деление под действием El-фотонов. При двухфотонном поглощении световой квант, практически не меняя энергии ядра, фактически меняет спин и четность основного состояния, и деление уже будет происходить под действием $E1$-квантов через состояние 2^+. Вероятность деления через канал 2^+увеличится в 17 раз и будет равна сечению деления через канал 1^-под действием $E1$-квантов.

9.

42. $\frac{w_{\text{дел}}\,(1^-}{w_{\text{дел}}\,(2^+)} = \frac{\sigma_{\text{дел}}\,(1^-)}{\sigma_{\text{дел}}\,(2^+)} D\,(\delta_\gamma) = \left(\frac{\hbar}{R_{\text{яд}}}\right)^2 \exp\left\{-\frac{2\pi(U_0-\mathscr{E}_\gamma)}{\hbar\omega}\right\} = 4,8,$ где $D\,(\mathscr{C}_\gamma)$ - проницаемость параболического барьера (см. задачу 3.41). См. также решение задачи 9.41 .

9.

43. $L_{\max} = \sqrt{\frac{(1-\alpha)W}{8\pi\Phi_0}} \leqslant 110$ км.

О3.1-9.23

В первом поколении термоядерных реакторов предполагается использовать реакцию дейтерия с тритием:

$$\mathrm{d} + \mathrm{t} \to {}^4\mathrm{He} + \mathrm{n}.$$

Теплота реакции $Q = 17,6$ МэВ. Предполагая, что квазинейтральная плазма содержит равное количество ядер дейтерия и трития при плотности электронов $n = 10^{14}$см$^{-3}$, рассчитать плотность тепловой мощности W, а также полную мощность N термоядерной установки. Объем плазмы $V = 500$ м ^{3}. Для данной реакции

$$\overline{\sigma v}_{\mathrm{dt}} = \begin{cases} 6,2\cdot 10^{-21}\text{см}^3/\text{с} & \text{при} \quad kT = 1, \\ 6\cdot 10^{-17}\text{см}^3/\text{с} & \text{при} \quad kT = 10 \text{ кэВ}. \end{cases}$$

9.

23. $W = n_{\mathrm{d}} n_{\mathrm{t}} \overline{\sigma v_{\mathrm{dt}}} Q_{\mathrm{dt}} = \frac{n^2}{4}\overline{\sigma n_{\mathrm{dt}}} Q_{\mathrm{dt}}$, где $n_{\mathrm{d}} = n_{\mathrm{t}} = n/2$. (См. задачу 9.20). $N = WV$.
При $kT = 1$ кэВ $\quad \boldsymbol{W} = 4,36\cdot 10^{-5}\text{В/см}^3, N = 21,8$ кВт.
При $kT = 10$ кэВ $W = 0,422\text{В/см}^3, N = 211$МВт.

О3.1-9.24

Термоядерная реакция называется самоподдерживающейся, если выделяемая энергия полностью уходит на разогрев плазмы (ядер дейтерия, трития и электронов) до необходимой темературы T. Исходя из этого, найти минимально необходимое время с удержания квазинейтральной дейтериево-тритиевой плазмы с полной концетрацией частиц $n_{\mathrm{d}} + n_{\mathrm{t}} = n$. Для данной реакции при данной температуре величины Q_{dt} и $\overline{\sigma v}_{\mathrm{dt}}$ считать заданными.

Пр и меч а н и е. Время удержания плазмы определяется в первую очередь различными неустойчивостями, а также процессами диффузии и излучения.

9.

24. $\tau \geqslant \frac{12kT}{\overline{\sigma v}_{\mathrm{dt}} n Q_{\mathrm{dt}}}$.

О3.1-9.25

Согласно критерию Лоусона в равнокомпонентной смеси дейтерия и трития при $kT = 10$ кэВ термоядерная реакция будет самоподдерживающейся, если $n\tau = 10^{14}\mathrm{c/cm}^{-3}$, где n - плотность элекетонов, т - время удержания плазмы (см. задачу 9.24). Какова для Этого случая должна быть плотность тепловой мощности, выделяемой в реакторе, если $n = 10^{14}\mathrm{см}^{-3}$.

П р и м е ч а н и е. Такой режим работы называют режимом нулевой мощности.

9.

25. $W_{\mathrm{выд}} = W_{\mathrm{нагр}} = \frac{3kTn^2}{n\tau} = 0,48\frac{\mathrm{Br}}{\mathrm{cm}^3}$.

9.26. $n\tau > \dfrac{36kT}{\overline{\sigma v_{\mathrm{dt}}} Q_{\mathrm{dt}}} \approx 3 \cdot 10^{14}\ \mathrm{с/см}^3$.

О3.1-9.26

Экономически выгодным считается такой термоядерный реактор, в котором выделяемая энергия втрое превышает затраты на ра- зогрев плазмы. Это связано с тем, что часть выделямой мощности должна идти на поддержание работы различных вспомогательных 85 устройств. Показать, что для квазинейтральной равнокомпонентной дейтериево-тритиевой плазмы при $kT = 10$ кэВ критерий Лоусона имеет вид $n\tau > 3 \cdot 10^{14}\mathrm{c/cm}^{-3}$. Здесь n - плотность электронов, т время удержания плазмы (см. задачу 9.24). Для данной реакции при заданной температуре $\overline{\sigma v_{\mathrm{dt}}} = 6 \cdot 10^{-17}\mathrm{см}^3/\mathrm{c}$, а $Q_{\mathrm{dt}} = 17,6\mathrm{МВ}$.

О3.1-9.27

Оценить радиус плазменного дейтериевого шара, для которого термоядерная реакция станет самоподдерживающейся при $kT = 10$ кэВ. Плазму можно рассматривать, как абсолютно черное тело, непрозрачное для излучения, и считать, что основные потери энергии связаны с излучением через поверхность шара. Концетрация дейтерия равна $n_{\mathrm{d}} = 3,0 \cdot 10^{20}\mathrm{см}^{-3}$; при данной температуре величина $\overline{\sigma v_{\mathrm{dd}}} = 10^{-18}\mathrm{см}^3/\mathrm{c}$. Учитывать только реакции (d,d) и (d,t) (см. задачу 9.20). Концентрации дейтерия и трития считать стационарными.

О3.1-9.28

При классическом рассмотрении реакция термоядерного синтеза (d,d) может произойти только тогда, когда кинетическая энергия сталкивающихся дейтронов достаточна для преодоления кулоновского барьера $U_{\mathrm{кул}} = 0,5$ МэВ. Однако, благодаря туннельному эффекту эта реакция возможна и при меньших энергиях. Оценить, во сколько раз увеличивается скорость реакции при квантовом рассмотрении по сравнению с классическим. Температура дейтериевой плазмы $T_0 = 10^8$ К.

О3.1-9.29

Реакция термоядерного синтеза $\mathrm{d}+\mathrm{t} \to \mathrm{n}+\alpha$ при низких энергиях идет преимущественно в состоянии с полным моментом импульса сталкивающихся ядер $I = 3/2$. Во сколько раз изменится среднее сечение этой реакции, если дейтериево-тритиевая плазма помещена в магнитное поле, полностью поляризующее спины взаимодей-

ствующих ядер? Спины ядер дейтерия и трития равны соответственно $S_{\mathrm{d}} = 1$ и $S_{\mathrm{t}} = 1/2$ (см. указание к задаче 8.4).

О3.1-9.30

В морской воде примерно на каждые 6000 молекул обычной воды приходится одна молекула тяжелой воды D_2O. Учитывая четыре основные реакции синтеза, возможные в дейтериевой плазме, определить, какая энергия выделится в термоядерном реакторе при сжигании всего дейтерия, содержащегося в 1 л морской воды. Какому количеству бензина эквивалентен по энергии 1 л воды, если при сжигании 1 кг бензина выделяется 13 кВт.ч энергии?

О3.1-9.31

Оценить запас термоядерной энергии $\mathcal{E}$ в 1 м ^{3} морской воды, если использовать 10% дейтерия, содержащегося в воде, для осуществления реакции $\mathrm{d}+\mathrm{d}$. Число атомов дейтерия в природной смеси изотопов равно $0,015\%$.

О3.1-9.32

Определить отношение начальной кинетической энергии частиц дейтериевой плазмы, нагретой до $T = 10^9$ К, к энергии, выделившейся после «выгорания» всего дейтерия в результате реакции термоядерного синтеза. Учитывать только реакции (d,d) и (d,t).

О3.1-9.33

На рис. 60 изображена предполагаемая схема термоядерной электростанции. В реактор вводится подогретое до необходимой температуры топливо - дейтериевая плазма. Часть частиц покидает зону реакции, не испытав ядерного взаимодействия. Часть энергии заряженных частиц, которая бесполезно излучается из зоны реакции за счет тормозного излучения, с помощью системы отражателей возвращается обратно в реактор. Коэффициент преобразования выделенной энергии в электрическую (КПД станции) $\eta = 30\%$ Температура дейтериевой плазмы $T = 10^9$ К. Найти $n_\mathrm{d}\tau$ - произведение концентрации ядер дейтерия на время удержания дейтериевой плазмы в зоне реакции, необходимое для протекания самоподдерживающейся реакции. Принять во внимание только реакции (d,d) и (d,t). При заданной температуре $\overline{\sigma v_{\mathrm{dd}}} = 2,5\cdot 10^{17}\text{см}^3\cdot\text{с}^{-1}$. Считать, что за единицу времени из единицы объема плазмы уходит в среднем n_d/τ частиц. Интенсивность тормозного излучения единицы объема $W_{\text{изл}} = 1,5\cdot 10^{-34} n_\mathrm{d}^2\sqrt{T}$ Вт/см. Для упрощения расчета принять, что доля β мощности потерь из-за тормозного излучения, возвращенная обратно в реактор отражателями, равна КПД станции, т.е. $\beta = \eta$.

О3.1-9.34

. Согласно современным представлениям на Солнце осуществляется звездный углеродный цикл, в результате которого из четырех протонов образуется $\alpha-$частица Конечной реакцией этого цикла является реакция $\mathrm{p} + {}^{15}\mathrm{N} \to {}^{12}\mathrm{c} + {}^4\mathrm{He}$. Оценить, какая доля энергии η от полной энергии цикла выделяется в указанной реакции.

О3.1-9.35

. Под действием медленных нейтронов из литиевой мишени, состоящей из изотопа 6 Li, вылетают тритоны. Они в свою очередь попадают в дейтериевую мишень и могут приводить к реакции $\mathrm{t}+\mathrm{d} \to \mathrm{n}+\boldsymbol{\alpha}$. Какова при этом максимальная кинетическая энергия вторичных нейтронов?

О3.1-9.36

Основная реакция в водородной среде в центрах звезд $\mathrm{p}+\mathrm{p} \to \mathrm{d}+\mathrm{e}^+ + v_\mathrm{e}$ обусловлена слабым взаимодействием. Этот процесс можно промоделировать в лабораторных условиях. Рассчитать, какой ток ϑ протонов с энергией 1 МэВ должен падать на водородную мишень, чтобы за $t = 1$ ч произошла одна такая реакция. Пробег протонов данной энергии в мишени до взаимодействия $l = 8\cdot 10^{-4}\text{г/см}^2$, сечение взаимодействия при данной энергии $\sigma = 10^{-47}\text{см}^2$.

О3.1-9.37

В центре Солнца плотность ядер водорода $\rho \approx 160$ г/см ^{3}, температура $T = 1,5\cdot 10^7$ К($kT \simeq 1$В). Рассчитать время выгорания 50% ядер водорода в центре Солнца за счет реакции $\mathrm{p}+\mathrm{p} \to \mathrm{d}+\mathrm{e}^+ + v_\mathrm{e}$. Считать, что все протоны в центре Солнца имеют скорость, равную скорости при данной температуре, а сечение их взаимодействия $\sigma = 10^{-51}\text{см}^2$.

О3.1-9.38

Сечение деления ядер ^{238}U составляет $\sigma = 0,1$ нбн $\left(10^{-34}\text{см}^2\right)$. Какова должна быть плотность потока $j\left[\text{см}^{-2}\cdot\text{с}^{-1}\right]$ падающих на мишень γ-квантов, чтобы можно было заметить вынужденное деление в $m = 1$ мг урана на фоне спонтанного деления $\left(T_{1/2} = 10^{15}\right.$ лет) при продолжительности эксперимента $t_0 = 100$ час?

О3.1-9.39

Оценить критический радиус и массу шара из металлического урана-235 плотностью $\rho = 18,7\text{g/cm}^3$ (заряда ядерной бомбы), если известно, что среднее сечение деления ядер рождающимися нейтронами $\sigma = 1,5$ бн, среднее число рождающихся в одном акте деления нейтронов $\upsilon = 2,5$. Всеми аругими каналами реакции, кроме делительного, пренебречь. Плотность потока нейтронов считать однородной.

18.2.9 Problems about nuclear fission and reactors 3

О3.1-9.40

В бесконечной среде, состоящей из металлического урана-235, самопроизвольно разделилось одно ядро. Коэффициент размножения нейтронов $k_\infty = 1,001$, средняя энергия делительных нейтронов $\mathscr{E} = 1,6\text{МВ}$, сечение деления этими нейтронами $\sigma = 1,5$ бн. Оценить. за какое впемя в среле выделится энергия $W = 5$ МДж. Плотность урана $\rho = 18,7\text{g/cm}^3$, неупругими процессами пренебречь.

О3.1-9.41

Высота и форма барьера деления зависят от спина (полного момента) и четности делящегося ядра (рис. 61). Так, например, в уране-238, у которого спин и четность основного состояния 0^+, высоты барьеров деления для возбужденных состояний ядра 2^+и 1^-равны 5,2 и 5,7 МэВ соответственно. Найти отношение β вероятностей деления ядра через эти состояния под действием γ - квантов с энергией $\mathcal{E}_\gamma = 6,0$ МэВ. Как изменится вероятность деления через состояние 2^+, если поместить ядра в поле интенсивного лазерного излучения (т. е. в случае, когда ядро практически одновременно поглощает γ-квант и фотон)?

О3.1-9.42

Высота и форма барьера деления зависят от спина (полного момента) и четности делящегося ядра (рис. 61). Так, например, у ядра ^{240}Pu, основное состояние есть 0^+, высоты барьеров деления для возбужденных состояний ядра
2^+и 1^-равны соответственно 5,2 и 5,7 МэВ. Оценить отношение вероятностей деления ядра через эти состояния под действием γ квантов с энергией $\mathcal{E}_\gamma = 5,4$ МэВ. Форму барьера деления для состояния 1^-можно аппроксимировать «перевернутой параболой» с характерным квантом $\hbar\omega = 1,3$ МэВ. См. также задачу 3.41.

О3.1-9.43

Источником питания находящегося на околоземной орбите спутника является ядерный реактор мощностью $W = 3$ кВт. Оценить, на каком максимальном расстоянии от спутника можно обнаружить наличие реактора с помощью γ-телескопа. Считать, что сигнал надежно регистрируется, если он вдвое превышает γ - фон неба $\Phi_0 = 10^{-2}\text{см}^{-2}\cdot\text{с}^{-1}$. В каждом акте деления в среднем испускается $k = 7$ γ-квантов, защита реактора поглощает $\alpha = 95\%$ образующегося излучения. Считать, что угловое разрешение телескопа равно угловому размеру спутника.

18.2.10 Basic Problems about Elementary Particles 1

О3.1-10.1

При рождении и распаде частиц выполняется (помимо законов сохранения энергии, импульса и момента импульса) ряд точных законов сохранения (тильда сверху в обозначении частицы является знаком античастицы): 1) Закон сохранения электрического заряда; 2) закон сохранения барионного заряда (барионный заряд равен 1 д.я барионов, т. е., например, для нуклонов (n, p) и гиперонов (Λ, Σ, Ξ); -1 для антибарионов, т. е., например, для антинукло (частиц); 3) законы сохранения электронного лептонного заряда L_e, мюонного лептонного заряда L_μ и таонного лептонного заряда L_τ. Для электрона (e^-)и электронного нейтрино (υ_e) принято, что $L_\text{e} = 1$, а для позитрона и электронного антинейтрино $L_\text{c} = -1$. Для всех остальных частиц $L_\text{e} = 0$. Аналогично, L_μ отлично от нуля только для четырех частиц: $\mu^-, \upsilon_\mu, \mu^+, \tilde{\upsilon}_\mu$ (мюонов и мюонных нейтрино), причем для первых двух частиц $L_\mu = 1$, а для последних

двух $L_\mu = -1$. Аналогично вводятся лептонные заряды и для сверхтяжелого лептона τ^-. Y какие из приведенных ниже реакций запрещены перечисленными законами сохранения: 1. $\to \mathrm{p} + \mathrm{e}^- + \tilde{v}_\mathrm{e}$ 5. $\pi^- + \mathrm{p} \to \Lambda^0 + \mathrm{K}^0$ 2. $\mathrm{p} \to n + \mathrm{e}^+$. 6. $\mathrm{K}^- + \pi \to \Lambda^0 + \pi^-$. 3. $\mu^- \to \mathrm{e}^- + v_\mu + \tilde{v}_\mathrm{e}$. 7. $\pi^+ + \Pi \to \Lambda^0 + K^+$. 4. $\mathrm{K}^+ \to \pi^- + 2\mathrm{e}^+$. 8. $\pi^+ + \mathrm{n} \to \mathrm{K}^+ + \mathrm{K}^0$.

O3.1-10.2

Рассмотреть приведенные ниже распады и реакции и указать, какие из них запрещены: 1. $\pi^- \to \mu^- + \tilde{v}_{\mu^*}$ 6. $\tilde{v}_\mu + \mathrm{p} \to \mathrm{n} + \mathrm{e}^+$. 2. $\pi^- \to \mu^- + \tilde{v}_{\mathrm{e}^*}$ 7. $\tilde{v}_\mathrm{e} + \mathrm{p} \to \mathrm{n} + \mu^+$. 3. $\mu^- \to \mathrm{e}^- + v_\mathrm{e} + \tilde{v}_\mathrm{e}$. 8. $\tilde{v}_\mathrm{e} + \mathrm{p} \to \mathrm{n} + \mathrm{e}^+$. 4. $\mu^- \to \mathrm{e}^- + \tilde{v}_\mathrm{e} + v_u$. 9. $\mu^- \to \mathrm{e}^- + \gamma$.

O3.1-10.3

Взаимодействие и распад частиц происходят в результате сильного, электромагнитного или слабого взаимодействий. Вероятность процессов при слабом взаимодействии на много порядков меньше, чем при сильном. Сильное взаимодействие может происходить только между адронами. При сильном и электромагнитном взаимодействиях сохраняется квантовое число S (странность). При слабом взаимодействии странность не сохраняется. Принято приписывать странность S частицам следующим образом: $S = 0$ аля нуклонов, антинуклонов, л-мезонов; 89 $S = -1$ для $\Lambda, \Sigma^+, \Sigma^-, \mathrm{K}^-, \Sigma^0, \tilde{K}^0$(K-мезонов, Σ-гиперонов, Λ - частицы);

$S = -2$ для Ξ^-, Ξ^0 (каскадных гиперонов);

$S = -3$ для $\Omega^-_\sim$(гиперона)

$S = +1$ для $\tilde{\Lambda}, \tilde{\Sigma}^+, \tilde{\Sigma}^-, \tilde{\Sigma}^0,\ \mathrm{K}^+, \mathrm{K}^0$

$S = +2$ для $\tilde{\Xi}^-, \tilde{\Xi}^0$;

$S = +3$ для Ω^+.

В этих формулах тильда сверху - знак античастицы. При изменении странности на 1 вероятность процесса уменьшается в $10^{10} \div 10^{12}$ раз по сравнению со случаем сильного взаимодействия, а при изменении S на 2 реакция фактически не наблюдается, если возможна реакция с изменением S только на 1. При существующей интенсивности частиц, генерируемых в ускорителях, реакции меж- ду ними с нарушением странности практически ненаблюдаемы. Олду ними с нарушением странности практически ненаблюдаемы. Однако распады частиц с нарушением закона сохранения странности наблюдаются всегда.

Выяснить, какие из перечисленных реакций и распадов разрешены по закону сохранения S, какие не наблюдаются:

1. $\pi^- + \mathrm{p} \to \Lambda + \mathrm{K}^0$. 8. $\pi^+ + \mathrm{n} \to \Lambda + \mathrm{K}^+$. 2. $\pi^- + p \to \Lambda + \pi^0$. 9. $\mathrm{K} + \mathrm{p} \to \Sigma^+ + \pi^+$. 3. $\Lambda \to \mathrm{p} + \pi^-$.

10. $\mathrm{p} + \tilde{\Sigma}^+ \to \mathrm{K}^+ + \pi^+$. 4. $\Xi^- \to \Lambda + \pi^-$. 11. $\mathrm{p} + \tilde{\Sigma}^+ \to \pi^+ + \pi^+$. 5. $\Xi^- \to 2\pi^- + \mathrm{p}$. 12. $\pi^- + \mathrm{p} \to \Xi^- + \Xi^+ + \mathrm{n}$. 6. $\pi^+ + \tilde{p} \to \underset{\tilde{\Sigma}^+}{} + \mathrm{K}^-$. 13. $\pi^- + \mathrm{p} \to \Sigma^+ + \mathrm{K}^-$. 7. $\pi^+ + \tilde{p} \to \tilde{\Sigma}^+ + \pi^-$. 14. $\pi^- + \mathrm{p} \to \Xi^- + \mathrm{K}^+ + \mathrm{K}^0$.

O3.1-10.4

При распадах странных адронов (барионов и мезонов), приводящих к рождению лептонов, существует эмпирическое правило, управляющее вероятностью распада. Если изменение странности адрона при реакции ΔS не равняется изменению заряда адронов ΔZ, то такой распад не наблюдается. Например, наблюдается распад

$$\Sigma^- \to \mathrm{n} + \mathrm{e}^- + \tilde{v}_\mathrm{e} (\Delta Z = \Delta S = +1),$$

но не наблюдается распад

$$\Sigma^+ \to \mathrm{n} + \mathrm{e}^+ + v_\mathrm{e} (\Delta Z = -1; \Delta S = +1).$$

Существование первого и отсутствие второго из этих распадов можно рассматривать как потверждение кварковой структуры адронов. Определить, какие из перечисленных ниже распадов разрешены по правилу $\Delta Z = \Delta S$, а какие запрещены:

1. $\mathrm{K}^+ \to \pi^+ + \pi^+ + \mathrm{e}^- + \tilde{v}_\mathrm{e}$.
6. $\Xi^0 \to \Sigma^+ + \mathrm{e}^- + \tilde{v}_\mathrm{e}$.
2. $\mathrm{K}^+ \to \pi^+ + \pi^- + \mathrm{e}^+ + v_\mathrm{e}$.
7. $\Xi^0 \to \Sigma^- + \mathrm{e}^+ + v_\mathrm{e}$.
3. $\Xi^- \to \Lambda + \mathrm{e}^- + \tilde{v}_{\mathrm{e}^-}$.
8. $\mathrm{K}^+ \to \mathrm{e}^+ + v_\mathrm{e} + \pi^0$.
4. $\Sigma^0 \to \Lambda + \mathrm{e}^- + \mathrm{e}^+$.
9. $\mathrm{K}^+ \to \pi^+ + \mu^+ + \mu^-$.
5. $\Lambda \to \mathrm{p} + \mathrm{e}^- + \tilde{v}_\mathrm{e}$.
10. $\mathrm{K}^- \to \pi^- + \pi^- + \mathrm{e}^+ + v_\mathrm{e}$.

О3.1-10.5

Все частицы естественным образом разбиваются на группы с близкими значениями масс (отличие масс в группе порядка 1%). Группу частиц с близкими массами называют изотопическим муль типлетом (синглетом, дублетом, триплетом, квартетом). Частицы мультиплета можно трактовать как различные состояния одной фиктивной частицы, отличающиеся значениями проекции нового квантового числа - изотопического спина T. Как и обычный спин (момент импульса), изотопический спин имеет $2T + 1$ проекций на ось квантования в фиктивном изотопическом пространстве. Число проекций изотопического спина совпадает с числом частиц в мультиплете, т. е. $N = 2T + 1$. При этом проекция изотопического спина на ось квантования T_3 связывается с электрическим зарядом члена мультиплета $T_3 = Z - Y/2$, где Y-квантовое число, одинаковое для всех членов мультиплета, называемое гиперзарядом (или унитарным спином). Поскольку $\Sigma T_3 = 0$, то $Y = 2\frac{Z}{N+1} = 2Z_{\text{ср}}$ - удвоенный средний заряд мультиплета. Оказалось, что странность S (см. задачу 10.3) связана с гиперзарядом Y и барионным зарядом B простым соотношением: $S = Y - B$. Пользуясь приведенными равенствами, определить S, T, T_3 и Y для $\Lambda, \Sigma^-, \Xi-, \Omega^-, \pi^-, \mathrm{K}^-$, η-частиц.

Пр и меч а ни е. Для античастиц все заряды (электрический, барионный, лептонный, гиперзаряд) противоположны зарядам частиц. Противоположны также странность S и проекция изотопического спина T_3. Массы, времена жизни, спины и изотопические спины T у частиц и античастиц совпадают. Частицы, у которых все заряды равны нулю, называются истинно нейтральными.

О3.1-10.6

Строгие законы сохранения (см. задачу 10.1) ограничивают число типов реакций и распадов. Нестрогие законы сохранения ограничивают типы взаимодействий. Какие из приведенных ниже реакций и распадов разрешены законами сохранения, какие строго запрещены, какие практически ненаблюдаемы? (См. задачу 10.3.)

1. $\mathrm{p} \to \mathrm{n} + \mathrm{e}^+ + v_{\mathrm{e}}$. 4. $\mu^- \to \mathrm{e}^- + \mathrm{e}^+ + \mathrm{e}^-$. 2. $\mu^- \to \mathrm{e}^- + \tilde{v}_{\mathrm{e}} + \gamma$. 5. $\mathrm{K}^+ + \Pi \to \Sigma^+ + \pi^0$. 3. $\pi^0 \to \mathrm{e}^- + \mathrm{e}^+ + \gamma$. 6. $\to \mathrm{p} + \mathrm{e}^- + \tilde{v}_{\mathrm{e}}$

О3.1-10.7

Указать, какие из перечисленных ниже реакций и распадов невозможны или практически ненаблюдаемы из-за нарушения законов сохранения: 1. $\Sigma^+ \to \pi^+ + \pi$. 5. $\pi^- + \mathrm{p} \to \Sigma^- + \mathrm{K}^+$. 2. $\Sigma^- + \mathrm{p} \to \pi^0 + \tilde{K}^0$. 6. $\Sigma^0 \to \Lambda + \gamma$ 3. $\pi^- + \mathrm{p} \to \Lambda + \tilde{K}^0$ 7. $\Sigma^- \to \Lambda + \mathrm{e}^- + \tilde{v}_{\mathrm{e}}$. 4. $\pi^- + \mathrm{p} \to \Sigma^+ + \mathrm{K}^-$. 8. $\Sigma^0 \to \pi^0 + \pi^0$. По какому типу взаимодействия происходят процессы $1, 5, 6, 7$?

О3.1-10.8

Рассмотреть приводимые ниже реакции и распады и определить тип взаимодействия:
1. $\mathrm{K}^- + \mathrm{p} \to \Lambda + \pi^0$. 4. $\Xi^0 \to \Lambda + \pi^0$ 2. $\pi^+ + \mathrm{p} \to \Sigma^+ + \mathrm{K}^+$ 5. $\pi^0 \to \gamma + \gamma$. 3. $\Sigma^0 \to \Lambda + \gamma$ 6. $\Omega^- \to \Xi^- + \pi^0$.

О3.1-10.9

Как отличаются друг от друга значения квантовых чисел K^0-мезона и $\tilde{K}^0$-мезона и как это сказывается на поглощении K^0 и $\tilde{\mathrm{K}}^0-$ мезонов веществом? Возможны ли переходы этих частиц друг в друга?

О3.1-10.10

Определить типы взаимодействий при следующих реакциях и распадах: 1. $\mathrm{K}^- + {}^4_2\mathrm{He} \to {}^3_2\mathrm{He} + \Lambda + \pi^-$. 5. ${}^4_2\mathrm{He} + {}^4_2\mathrm{He} \to {}^6_3\mathrm{Li} + {}^2_1\mathrm{H} + \pi^0$. 2. ${}^2_1\mathrm{H} + {}^2_1\mathrm{H} \to {}^4_2\mathrm{He} + \pi^0$. 6. $\Omega^- \to \mathrm{K}^- + \Lambda$. 3. $\mathrm{p} + {}^4_2\mathrm{He} \to {}^3_2\mathrm{He} + {}^2_1\mathrm{H}$. 7. $\pi^- \to \mu^- + \tilde{v}_\mu$. 4. ${}^3_2\mathrm{He} + {}^3_1\mathrm{H} \to {}^4_2\mathrm{He} + {}^2_1\mathrm{H}$. 8. $\mathrm{n} \to \mathrm{p} + \mathrm{e}^- + \tilde{v}_{\mathrm{e}}$.

О3.1-10.11

Возможны ли следующие схемы распада частиц, и если нет, то по какой причине? 1. $\Omega^- \to \Lambda^0 + \pi^-$. 4. $\mathrm{n} \to \mathrm{p} + \mathrm{e}^- + \tilde{v}_{\mu^*}$ 2. $\Xi^- \to \mathrm{n} + \pi^-$. 5. $\mathrm{p} \to \mu^+ + \tilde{v}_\mu$. 3. $\mathrm{n} \to \mathrm{p} + \mu^- + \tilde{v}_\mu$. 6. $\Omega^- \to \Xi^0 + \mu^-$.

О3.1-10.12

Какая частица обязана образоваться одновременно с K^0 - мезоном при соударении π^--мезона с протоном? Реакция идет по сильному взаимодействию.

О3.1-10.13

«Эспериментом века» были названы опыты по определению времени жизни протона. Теория великого объединения предсказывает, что протон распадается на пион и лептоны со временем жизни $\tau \sim 10^{31}$ лет. Оценить, какую массу вещества необходимо использовать, чтобы за время эксперимента $t = 1$ год произошло $N = 10$ таких распадов.

О3.1-10.14

Определить время жизни мюона, образовавшегося при распаде положительно заряженного каона. До распада каон покоился.

О3.1-10.15

Определить время жизни ипсилон-частицы Υ по ширине ее резонанса $\Delta\mathscr{E}$, взятой на половине высоты и равной 25 кэВ.

О3.1-10.16*

Найти, какие из самых тяжелых ядер и антиядер могут образоваться в реакции $\mathrm{p} + \mathrm{p}$ при соударении протона с энергией протонов, ускоренных до такой же энергии.

О3.1-10.17

В 1976 г. Нобелевская премия по физике была присуждена за открытие новой элементарной частицы - джи-мезона (ныне: J/ψ-мезон). Открытие было сделано практически одновременно и независимо в двух разных лабораториях. В одной из них опыт был поставлен на встречных пучках электронов и позитронов, ускоренных до одинаковой энергии $_{\text{сцм}}$ ($\mathscr{E}_{\text{сцм}}$ - энергия сталкивающихся частиц в системе центра масс). Полученные в этом эксперименте результаты показаны на рис. 62. Определить энергию покоя и оценить нижнюю границу времени жизни джи-частицы.

О3.1-10.18

В 1984 г. появилось сообщение, впоследствии не подтвердившееся, об открытии реакции $\Upsilon \to \xi + \gamma$. Определить энергию покоя и скорость гипотетической ξ-частицы в системе покоя Υ-частицы, если энергия γ-кванта в этой системе оказалась $\mathscr{Q}_\gamma = 1072$ МэВ. Энергия покоя Υ-частицы равна $m_\Upsilon c^2 = 9460$ МэВ.

О3.1-10.19

В 1974 г. была открыта элементарная частица J/ψ, названная впоследствии чармонием. В одном из опытов были зарегистрированы продукты ее распада «на лету»: $\mathrm{J}/\psi \to \mathrm{e}^+ + \mathrm{e}^-$. Найти
массу и скорость чармония, если энергии и электрона, и позитрона были равны $\mathcal{E} = 3,1$ ГэВ, а угол между направлениями разлета электрона и позитрона составил $\theta = 60°$.

О3.1-10.20

В 1976 г. были получены первые указания о существовании заряженной «очарованной» $\tilde{\Lambda}_c^-$ частицы, распадающейся по схеме

$$\tilde{\Lambda}_\mathrm{c}^- \to \tilde{\Lambda} + \pi^- + \pi^+ + \pi^-.$$

Найти кинетическую энергию, уносимую продуктами распада $\tilde{\Lambda}_c^-$-частицы в ее системе покоя.

О3.1-10.21

Определить, выше какой минимальной энергии $_{\min}$ встречных электрон-позитронных пучков, имеющих одинаковую энергию, могут рождаться частицы из семейства «красивых» (B-мезоны). Энергия покоя B-мезона $m_\mathrm{B}c^2 \approx 5279$М.

О3.1-10.22

Определить пороговую энергию $\mathscr{E}_{\text{пор}}$ рождения пары Σ-гиперонов при облучении протонами жидководородной мишени.

О3.1-10.23

Найти, чему равно наибольшее количество заряженных или нейтральных пионов, которое может быть образовано при столкновении протона с энергией $\mathscr{E}_p = 5$ ГэВ с покоящимся протоном. 93

О3.1-10.24

Определить минимальную (пороговую) кинетическую энергию нейтрона, при столкновении которого с ядром водорода в Жидководородной мишени образуется лямбда-частица.

О3.1-10.25

Найти минимальную (пороговую) кинетическую энергию налетающего протона, необходимую для рождения пары барионов $\left(\Xi^0\widetilde{\Xi}^0\right)$, имеющих энергию покоя по 1315 МэВ дарениях в жидководородной камере.

О3.1-10.26

Определить максимальную энергию $\mathscr{E}_{\max}$ электрона, образующегося при распаде покоящегося мюона.

О3.1-10.27

Определить в лабораторной системе отсчета минимальную и максимальную энергии электрона, образованного при распаде мюона с энергией 10.5 ГэВ.

О3.1-10.28

Нейтральный пион распался на два γ-кванта с энергиями $\mho_1 = 3,1$ и $\sigma_2 = 2,0$ ГэВ. Найти угол разлета θ между γ-квантами.

О3.1-10.29

Оценить, при какой энергии $\mathfrak{o}$ ультрарелятивистского заряженного пиона его пробег до распада равен пробегу в воздухе при плотности $\rho = 10^{-5}\mathrm{g/cm}^3$. Собственное время жизни и энергия покоя пиона равны $\tau_0 = 2,6 \cdot 10^{-8}$ с и $m_\pi c^2 = 140\mathrm{M}$.

О3.1-10.30

Нейтральный пион π^0с энергией покоя $m_\pi c^2 = 135\mathrm{MB}$ распадается на лету на два одинаковых γ-кванта, разлетающихся под углом $\alpha = 2 \cdot 10^{-2}$ рад по отношению к направлению движения пиона. Какова кинетическая энергия пиона π^0? Чему равна неопределенность энергии покоя пиона π^0 и каково его время жизни в лабораторной системе координат, если в собственной системе он живет $\tau_0 = 0,84 \cdot 10^{-16}$с?

О3.1-10.31

D^0-мезон распадается на лету на K^-−и $^+$−мезоны. Расстояние от точки его рождения до точки распада равно $L = 350$ мкм. Импульсы каона и пиона равны $p_K = 3,6\Gamma$ В/c и $p_\pi = 1,9\Gamma$ В/c и направлены под углами $\theta_\mathrm{K} = 13°30'$ и $\theta_\pi = 27°50'$ к направлению импульса D^0-мезона. Определить энергию покоя, скорость и время жизни D^0 −

О3.1-10.32

* При распаде «на лету» Ω^--гиперона $(\Omega^- \to \Lambda + \mathrm{K}^-)$измерены импульсы частиц распада $p_\Lambda = 5,7\Gamma\Xi/c$ и $p_\mathrm{K} = 2,0\Gamma$ В/с и угол разлета между ними $\theta = 28,5°$. Определить энергию покоя Ω^--гиперона.

О3.1-10.33

За распадом остановившегося в ядерной фотоэмульсии K^+ мезона по схеме $\mathrm{K}^+ \to \pi^+ + \pi^0$ последовал распад нейтрального пиона π^0 по схеме $\pi^0 \to \gamma + \mathrm{e}^+ + \mathrm{e}^-$, причем точка рождения пары $\mathrm{e}^+\mathrm{e}^-$находилась на расстоянии $L = 0,04$ мкм от места остановки К-мезона. Оценить собственное время жизни нейтрального пиона π^0.

О3.1-10.34

Какова средняя длина пути L до распада Λ-гиперона в воздухе, если его энергия $E_A = 7$ ГэВ?
(их еще просто дохрена, лень выгружать.)

Рассеяние электрона на неподвижном литии++

дана энергия лития.
у лития один свободный электрон, знать типа нужно и что у лития $Z = 3$
минимальная возможная энергия электрона после взаимодействия?
рассматривать нужно неупругое рассеяние, ибо так она теряется больше.
масса лития на много порядков больше массы электрона
нужно разобраться, какую максимальную энергию может отдать электрон литию.
посмотрим, куда может перейти электрон?
а очень просто, мы смотрим на разницу уровней, один первый уровень - при $n = 1$, тогда для второго уровня подбираем n_2 такое, чтобы хватило энергии электрона, то есть разница энергий должна быть менее энергии электрона. так и находим, сколько он может отдать.
(интересно, а через теорию рассеяния кавнтмеха если сделать, что будет?)

10. Элементарные частицы. Резонансы. Лептоны и кварки. Реакции при высоких энергиях

10.

1. Запрещены распады 2 и 4 , так как не сохраняется лептонный заряд, и распад 8, так как не сохраняется барионный заряд; в распаде 2 нарушается еще закон сохранения энергии.

10.

2. Распады $2, 3, 9, 10$ и реакции 6,7 запрещены, так как в них не сохраняется лептонный заряд. При изучении взаимодействия нейтрино, полученных в распаде 1 , с протонами было показано, что идет реакция 5 , а не 6, хотя последняя энергетически более выгодна. Тем самым было доказано существование двух типов нейтрино.

10.

3. В реакциях $1, 6, 8, 10, 12, 14|\Delta S| = 0$, и они идут по сильному взаимодействию с характерными временами $10^{-22} \div 10^{-24}$ с (ядерные времена). В реакциях $2, 7, 9, 11|\Delta S| = 1$, и они практически ненаблюдаемы. В распадах 3 и $4|\Delta S| = 1$, и они идут по слабому взаимодействию с характерными временами $\sim 10^{-10}$ с. В процессах 5 и $13|\Delta S| = 2$, и поэтому такие процессы не наблюдаются.

10.

4. По указанному правилу разрешены распады $2, 3, 4, 5, 6, 8$; запрещены распады $1, 7, 9, 10$.

10.

5. 1. Барион Λ - синглет с зарядом $Z = 0$. Следовательно, $N = 1$, $T = 0, Z_{\text{ср}} = 0, S = -1, Y = 0, T_3 = 0$.
2. Барион Σ - триплет с зарядом ± 1 и 0 . Следовательно, $Z_{\text{ср}} = 0$, $N = 3, T = 1, Y = 0, S = -1, T_3 = Z$.
3. Барион Ξ - дублет с зарядами 0 и -1. Следовательно, $N = 2$, $T = 1/2$, $Z_{\text{ср}} = -1/2$, $S = -2$, $Y = -1$, $T_3 = -1/2$ для $Z = -1$ и $T_3 = \pm 1/2$ для $Z = 0$.
4. Отрицательно заряженный барион Ω^-- синглет. Следовательно, $N = 0, Z_{\text{ср}} = -1, S = -3, Y = -2, T = 0, T_3 = 0$.
5. Мезон л с зарядами $\pm 1, 0$. Следовательно, $N = 3, T = 1, T_3 = Z$, $S = 0, Y = 0$. Заметим, что если в составе мультиплета имеется истинно нейтральная частица, то при вычислении числа частиц в мультиплете N нужно вместе считать частицы и античастицы. Во всех других случаях под N подразумевается число частиц.
6. Мезон K - дублет с зарядами 0 и +1 . Следовательно, $N = 2$, $Z_{\text{ср}} = 1/2, S = 1, T = 1/2, T_3 = 1/2$ для K^+и $T_3 = -1/2$ для K^0.
7. Мезон η - нейтральный синглет. Следовательно, $N = 1, T = S = Z_{cp} = T_3 = 0$.

10.

6. Распады 2 и 4 запрещены законом сохранения лептонного заряда. Реакция 5 практически ненаблюдаема из-за несохранения странности. Распад 3 и 6 разрешены. Распад 1 запрещен законом сохранения энергии.

10.

7. Реакция 2 и распад 8 невозможны, так как не сохраняется барнионный заряд. Реакции 3 и 4 практически ненаблюдаемы из-за несохранения странности. Распады 1 и 7 происходят по слабому взаимодействию, распад 6 - по электромагнитному. Реакция 5 происходит по сильному взаимодействию.

10.

8. Реакции 1 и 2 происходят по сильному взаимодействию; распады 3 и 5 - по электромагнитному; 4 и 6 - по слабому взаимодействию.

10.

9* Странность K^0-мезона равна +1 , а странность $\tilde{K}^0$-мезона равна -1. Поскольку странность нуклонов равна 0, а странность других барионов либо равна нулю, либо отрицательна, то поглощение $\tilde{K}^0$-мезона может происходить с сохранением странности, т. е. по сильному взаимодействию. Погло-

щение K^0-мезона может происходить лишь с несохранением странности, т. е. по слабому взаимодействию. Следовательно, K^0-мезон в отличие от $\tilde{K}^0$ будет слабо поглощаться веществом. Поскольку при переходах $K^0 \rightleftarrows K^0 |\Delta S| = 2$, то такие переходы крайне маловероятны (см. задачу 10.3).

10.10.

Реакции $1, 3, 4$ происходят по сильному взаимодействию; распады $6, 7, 8$ - по слабому; реакции 2 и 5 - по электромагнитному взаимодействию.

10.

11. 1. Так как $\Delta S = 2$, то возможна, но маловероятна.
2. Так как $\Delta S = 2$, то возможна, но маловероятна.
3. Нет, так как $(m_\text{n} - m_\text{p}) < m_\mu$.
4. Нет, не сохраняется лептонный заряд.
5. Нет, не сохраняется барионный заряд.
6. Нет, не сохраняется лептонный заряд.

10.

12. Λ-гиперон или Σ^0-гиперон.

10.

13. $M = m_\text{n} N \frac{\text{t}}{t} \approx 170$ т, где $m_\text{n} \approx 1,7 \cdot 10^{-24}$ г - масса нуклона.

10.

14. $\tau = \frac{\mathscr{E}_\mu \tau_0}{m_\mu c^2} = 5,4$ мкс, где τ_0 - собственное время жизни мюона, $\mathscr{E}_\mu = \frac{m_{\mathrm{K}}^2 c^4 + m_\mu^2 c^4}{2 m_{\mathrm{K}} c^2}$.

10.

15. $\tau \sim \frac{\hbar}{\Delta \S} \approx 2,6 \cdot 10^{-20}$с.

10.

16* 1. $A = 38$ (на неподвижной мишени). 2. $A \approx 3000$ (на встречных пучках), т. е. все известные ядра.

Решение. Найдем сначала скорость центра масс системы. Пусть энергия налетающей частицы $\mathscr{E}_1$, а покоящейся $m_2 c^2$. Суммарная энергия системы $\mathscr{E} = \mathscr{E}_1 + m_2 c^2$. Полный импульс системы $\mathbf{p}_1$. Рассматривая эту систему как сложную частицу, находим скорость центра масс

$$\frac{\mathbf{v}_{\mathrm{LL,M.}}}{\boldsymbol{c}} = \frac{\mathbf{p_I c}}{\mathfrak{E}_1 + m_2 c^2}.$$

Энергии частиц в системе центра масс (СЦМ) равны

$$\mathscr{E}_1^* = \frac{\mathscr{E}_1 - \mathbf{p}_1 \mathbf{v}_{\text{ц. м.}}}{\sqrt{1 - (v_{\text{ц. м}}/c)^2}}; \quad \mathscr{E}_2^* = \frac{m_2 c^2 - 0}{\sqrt{1 - (v_{\mathrm{L.}}/c)^2}}.$$

Таким образом, суммарная энергия в СЦМ

$$\mathscr{E}_{\mathrm{L,M.}}^* = \mathscr{E}_1^* + \mathscr{E}_2^* = \sqrt{m_1^2 c^4 + m_2^2 c^4 + 2 m_2 c^2 \mathscr{E}_1},$$

где было использовано релятивистское выражение для полной энергии частицы

$$\mathscr{E}_1^2 = (p_1 c)^2 + \left(m_1 c^2\right)^2.$$

Эту формулу можно было бы получить и без преобразований Лоренца, считая, что две частицы в СЦМ рождают одну с массой $Mc^2 = \mathfrak{E}_{\text{ц. м.}}^*$. Исполь-

зуя инвариант, получим $\left(Mc^2\right)^2 = \mathscr{E}_{\text{ц. м.}}^2 - 0^2 = \left(\mathscr{E}_1 + m_2 c^2\right)^2 - p_1^2 c^2 = \left(\mathscr{E}_1 + m_2 c^2\right)^2 - \left[\mathscr{E}_1^2 - \left(m_1 c^2\right)^2\right]$, откуда следует то же выражение

$$\mathscr{E}_{\mathrm{L,M.}}^* = \sqrt{m_1^2 c^4 + m_2^2 c^4 + 2 m_2 c^2 \mathscr{E}_1}$$

Для двух одинаковых частиц $m_1 = m_2 = m_{\mathrm{p}}$ получаем

$$\mathrm{p} + \mathrm{p} \to \mathrm{M} + \tilde{\mathrm{M}} + \mathrm{p} + \mathrm{p}$$

и $\mathscr{E}_{\mathrm{L,M.}}^* = \sqrt{2 m_{\mathrm{p}} c^2 \left(\mathscr{E}_1 + m_{\mathrm{p}} c^2\right)}$.

Очевидно, что $\mathscr{E}_{\text{н. м.}}^* \geqslant \left[2 A m_{\mathrm{p}} + 2 m_{\mathrm{p}}\right] c^2$, откуда $2 m_{\mathrm{p}} c^2 \mathscr{E}_1 + 2\left(m_{\mathrm{p}} c^2\right)^2 \geqslant \geqslant 4\left(m_{\mathrm{p}} c^2\right)^2 (A+1)^2$. Если учесть, что $\mathscr{E}_1 \gg m_{\mathrm{p}} c^2$, то получим ответ в первом случае (столкновения с неподвижным протоном)

$$A \lesssim \sqrt{\frac{1}{2 m_{\mathrm{p}} c^2}} - 1 \lesssim 39, \text{ т. е. } A = 38 \text{ (включительно).}$$

На встречных пучках

$$2\mathscr{E}'' = 2 A m_{\mathrm{p}} c^2 + 2 m_{\mathrm{p}} c^2 \approx 2 A m_{\mathrm{p}} c^2$$

откуда $A \approx 3000$, т.е. практически все известные ядра.

10.

17* $\tau \approx 3 \cdot 10^{-22}$с; $mc^2 \approx 3,1$ ГэВ.

Решение. Масса частицы в данном случае равна $\mathscr{E}_{\text{сцм}}$, соответствующей положению максимума на графике. Полуширина резонансной кривой на уровне $1/2$ высоты $\Delta\mathscr{E} \approx 2$М В. Время жизни находим из соотношения неопределенностей $\tau \approx \hbar/\Delta\mathscr{E} \approx 3 \cdot 10^{-22}$ с.

10.

18. $m_\xi c^2 = \sqrt{m_Y c^2 \left(m_Y c^2 - 2\mathscr{E}_\gamma\right)} = 8,32$ ГЭВ, $\beta = \frac{\mathscr{E}_\gamma}{m_\gamma c^2 - \mathscr{E}_\gamma} \approx 0,13$.

10.

19. $m_{J/\Psi} c^2 = \mathscr{E}\sqrt{2(1-\cos\theta)} = 3,1$ ГЭВ; $\beta = \sqrt{\frac{1+\cos\theta}{2}} = \frac{\sqrt{3}}{2} \approx 0,87$.

10.

20. $T \approx 751$М В .

10.

21. $\mathscr{E}_{\min} \geqslant 2m_{\mathrm{B}}c^2 \approx 10,56$ ГэВ.

10.

22. $_{\text{пор}} = 4m_\Sigma c^2 + m_{\mathrm{p}}c^2 + 2\frac{m_\Sigma^2}{m_{\mathrm{p}}}c^2 = 8,8$ ГэВ.

10.

23. $N_{\max} = \frac{\sqrt{2m_{\mathrm{p}}c^2(\varrho_{\mathrm{p}}+m_{\mathrm{p}}c^2)}-2m_{\mathrm{p}}c^2}{2m_{\mathrm{r}}c^2} = 5,2$ (пар пионов), всего может родиться не более 10 пионов.

10.

24. $T_{\text{пор}} = \frac{(m+M)^2-(2m)^2}{2m}c^2 = 1,6$ ГэВ, где $m_{\mathrm{p}} \approx m_{\mathrm{n}} = m$; $M = m_\Lambda + m_{\mathrm{K}}$, где m_{K} - масса либо K^0-, либо K^+-мезона.

10.

25. $T_{\text{пор}} = 8,94$ ГэВ.

10.

26. $\mathscr{E}_{\max} = \frac{m_\mu c^2}{2}\left(1 + \frac{m_{\mathrm{e}}^2}{m_\mu^2}\right) \approx \frac{m_\mu c^2}{2} \approx 52,8$М э В.

10.

27. $\mathscr{E}_{\min} = m_{\mathrm{e}}c^2 \simeq 0,5$М ВВ $\mathscr{E}_{\max} \simeq \mathscr{E}_\mu - \frac{m_\mu^2 c^4}{2\mathscr{E}_\mu} \approx 10,5$ ГэВ.

10.

28. $\sin\frac{\theta}{2}=\frac{m_\pi c^2}{2\sqrt{\varepsilon_1\varepsilon_2}}=0,027.$

10.

29. $\mathscr{E}=m_\pi c^2\frac{2A_{\mathrm{N}}}{c\tau\rho N_{\mathrm{A}}\sigma}\approx 1,4$ Т ТВ, где A_{N} - атомная масса азота, $\sigma=2\pi R_{\mathrm{N}}^2$ - сечение рассеяния быстрых пионов, равное удвоенному геометрическому сечению ядра, $R_{\mathrm{N}}=1,3\cdot 10^{-13}A_{\mathrm{N}}^{1/3}$.

10.

30. $T=6,615$ ГэВ; $\delta\&\approx 7,8\ni$ В; $\tau=4,2\cdot 10^{-15}$с.

10.

31. $m_{\mathrm{D}}\mathrm{c}^2\approx 1,85\Gamma\ni$ В; $\beta=0,94;\tau\approx 4,2\cdot 10^{-13}$с.

10.

32: $m_\Omega c^2\approx 1,7$ ГэВ.

Решение. Для нахождения массы Ω^--гиперона воспользуемся инвариантностью квадрата четырехимпульса

$$m_\Omega^2c^4=\left(\mathscr{E}_1+\mathscr{E}_2\right)^2-\left(\mathbf{p}_1+\mathbf{p}_2\right)^2c^2$$

Нетрудно видеть, что Λ^0-гиперон и K^0-мезон можно считать ультрарелятивистскими, поскольку массы этих частиц малы по сравнению с произ ведениями pc : $m_\Lambda c^2\approx 1,1$ ГэВ; $m_\kappa c^2\approx 0,49$ ГэВ (табличные данные). Поэтому $\mathscr{E}_1\approx p_1c;\mathscr{E}_2\approx p_2c$. Раскрывая скобки, получим $m_\Omega^2c^4\approx 2\mathscr{E}_1\mathscr{E}_2$ - $-2p_1p_2c^2\cos\theta\approx 2p_1p_2c^2(1-\cos\theta)$, откуда

$$m_\Omega c^2\approx 2\sqrt{p_\Lambda p_{\mathrm{K}}}c\sin\frac{\theta}{2}=1,68\ \text{ В}\approx 1,7\text{ ГэВ}.$$

10.

33. $\mathrm{T}_0\approx 0,88\cdot 10^{-16}$с, $\beta=0,835$.

10.

34. $L=\frac{c\tau_{0\Lambda}}{m_\Lambda c^2}\approx 50$ см, где $\tau_0\approx 2,66\cdot 10^{-10}$с; $m_\Lambda c^2=1116$ МэВ.

18.2.11 Basic Problems about Elementary Particles 2

other solutions, I'll add problems later

10.

35: $L=(2\ln 2)\frac{c\tau_0\lambda\!\!\!^{-}_\pi}{m_\pi c^2}=770$ m, где $\mathbf{t}_0=2,6\cdot 10^{-8}$с; $m_\pi c^2\approx 140$М МВ .

Решение. За период полураспада $T_{1/2}$ пиона (по схеме $\pi^+\to\mu_++\upsilon_\mu$) половина пионов переходит в мюоны. Еще через $T_{1/2}$ число мюонов в потоке превышает число пионов в три раза. Таким образом, искомая длина $L=\upsilon_\pi 2T_{1/2}\gamma$, где $\gamma=\frac{1}{\sqrt{1-\beta^2}}=\frac{\lambda\!\!\!^{-}_\pi}{m_\pi c^2}$.

Скорость пионов v_π близка к скорости света, поскольку $\mathscr{E}_\pi \gg m_\pi c^2$. Период полураспада $T_{1/2} = \tau_0 \ln 2$, где τ_0 - собственное время жизни π^+ ($\boldsymbol{\tau}_0 = 2,6 \cdot 10^{-8}$с). Окончательно

$$L \approx (2 \ln 2) \frac{c_0 \mathscr{E}_\pi}{m_\pi c^2} \approx 770\text{М}.$$

Можно решить задачу иначе. Поскольку $\mathscr{E}_\pi = 10$ ГэВ $\gg m_\pi c^2$, то пионы можно считать ультрарелятивистскими. Мюоны, вылетающие в направлении движения пионов, также имеют скорость $v \approx c$. Собственное время жизни мюона примерно в 100 раз больше времени жизни пиона. Поэтому распадом мюонов в данной задаче пренебрегаем. Тогда $N_\pi(x) + N_\mu(x) = N_\pi(0)$. По закону радиоактивного распада

$$dN_\pi(x) = -\lambda N_\pi(x) dt = -\frac{N_\pi(x)}{\tau} dt.$$

Здесь $\tau = \gamma\tau_0 = \tau_0 \frac{\varrho_\pi}{m_\pi c^2}$, а $vdt = cdt = dx$, откуда $\frac{dN_\pi(x)}{dx} = -N_\pi \frac{m_\pi c^2}{\varrho_\pi \tau_0 c}$ или $N_\pi(x) = N_\pi(0) \exp\left(-\frac{m_\text{п} c^2}{\mathscr{E}_\pi c_0} x\right)$. По условию $3N_\pi(L) = N_\mu(L)$, поэтому $4 \exp\left(-\frac{m_\pi c^2}{\pi c_0} L\right) = 1$, откуда и следует приведенный выше ответ задачи.

10.

36. $\frac{N_\mu(L)}{N_\text{К}(0)} = 1 - \exp\left(-\frac{m_\text{К} c^2}{\mathscr{E}_\text{К}} \frac{L}{v\tau_0}\right) = 0,364$, где $\tau_0 = 1,24 \cdot 10^{-8}$с - время жизни $K^\pm$.

10.

37. $\frac{N_\mu(L)}{N_\text{К}(L)} \simeq 1800$.

10.

38. $\mathscr{E}_\mu = \frac{m_\pi^2 c^4 + m_\mu^2 c^4}{2 m_\pi c^2} \cdot \frac{\mathscr{E}_\pi}{m_\pi c^2} \approx 330\text{М} \ni \text{В}$.

10.

39: $N_\pi \approx 3,6 \cdot 10^7$ частиц/с.

Решение. Число пионов, достигших детектора, $-n = \frac{N_\pi}{4\pi} \Omega e^{-t/\tau}$, где N_π - число всех генерированных пионов, $\Omega = S/L^2$ - телесный угол, под которым виден детектор из точки генерации пионов, t - время пролета пионом пути L, т - время жизни пиона в лабораторной системе отсчета:

$$\tau = \frac{\tau_0}{\sqrt{1-\beta^2}} = \tau_0 \frac{\mathscr{E}}{m_\text{а} c^2} = \tau_0 \left(1 + \frac{T}{m_\pi c^2}\right).$$

Окончательно получаем

$$N_\pi = n \frac{4\pi L^2}{S} \exp\left(\frac{L}{c\tau_0} \frac{m_\pi c^2}{\sqrt{T^2 + 2 m_\pi c^2 T}}\right) \approx 3,6 \cdot 10^7 \frac{\text{частиц}}{c}.$$

10.

40. $\mathscr{E}_\text{пор} = (m_\text{п} - m_\text{р} + m_\text{е}) c^2 \approx 1,8\text{М} \ni \text{В}$.

10.

41. $\mathscr{E}_{\mathrm{e}}^{\max} \approx \mathscr{E}_{\mu}^{\max} \approx \frac{\left(m_{\mathrm{e}}c^2\right)^2+\left(m_{\mu}c^2\right)^2}{2m_{\tau}c^2} \approx 0,9$ ГэВ. Точнее: $\mathscr{E}_{\mu}^{\max} \approx \frac{m_{\tau}c^2}{2} \times \times \left[1+\left(m_{\mu}/m_{\imath}\right)^2\right] = 0,894$ ГЭВ , $\mathscr{E}_{\mathrm{e}}^{\max} \approx \mathscr{E}_{\mu}^{\max}\left[1-\left(\frac{m_{\mu}c^2}{2\mathscr{E}_{\mu}^{\max}}\right)^2\right] = 0,891$ ГЭВ.

10.

42. $T = m_{\pi}c^2 \frac{2(m_{\mathrm{p}}+m_{\mathrm{n}})+m_{\pi}}{2(m_{\mathrm{p}}-m_{\pi})} \approx 330$М3 В.

10.

43. $\mathscr{E}_{\mathrm{p}} = m_{\mathrm{p}}c^2 \simeq 1$ ГЭВ.

10.

44. $\mathscr{E}_{\mathrm{p}} = m_{\mathrm{p}}\mathrm{c}^2 \frac{T}{2\varepsilon} = 6,57 \cdot 10^{19}$ДВ; $\tau \approx \frac{1}{n\sigma c} \approx 10^{15}\mathrm{c} \sim 3 \cdot 10^7$ лет.

10.

45. $T \approx 2,6 \cdot 10^{14} \ni$ В; $\tau \approx 8 \cdot 10^{10}$с.

10.

46. $\mathscr{E}_{\mu} = m_{\mu}c^2 \frac{H}{\tau_0 c} \approx 6,4$ ГЭВ.

10.

47. $\mathscr{E}_{\min} = \Delta\mathscr{E} \approx \rho\alpha H \simeq 9$ ГэВ, где $\Delta\mathscr{E}$ - потери энергии на ионизацию.

10.

48. $\frac{\delta T_{\mu}}{T_{\mu}} = \left(\frac{m_v}{m_{\pi}-m_v}\right)^2 \approx \begin{cases} 0,15 \cdot 10^{-4} \text{ при } m_v c^2 = 0,17\text{М МВ} , \\ 0,86 \cdot 10^{-5} \text{ при } m_v c^2 = 0,1 \text{ МэВ}. \end{cases}$

10.

49. Выход мюонных антинейтрино (нейтрино) составляет $2,0002\%$ от числа пионов. Выход электронных антинейтрино (нейтрино) составляет $0,0002\%$ от числа пионов.

10.

50. Процесс рассеяния нейтрино на электронах - это тот же Комп-тон-эффект (рассеяние фотонов на электронах):

$$\mathscr{E} = \frac{T_{\mathrm{e}}+pc}{2} = \frac{\left[T_{\mathrm{e}}+\sqrt{T_{\mathrm{e}}\left(T_{\mathrm{e}}+2m_{\mathrm{e}}c^2\right)}\right]}{2} = 5,24\text{М} \ni \text{ В}.$$

10.

51. $\cos\beta = \frac{T_e\left(\mathscr{E}+m_e c^2\right)}{\mathscr{E}\sqrt{T_e(T_e+2m_e c^2)}} = 0.927; \beta \approx 22^\circ$ (для $\mathscr{E} = 15$М В).

10.

52. $\frac{\Phi(v_\mu)}{\Phi(v_e)} = 2$. Наблюдение потоков атмосферных нейтрино на установке Super-Kamiokande не подтверждает этот результат. Таким образом, следует признать факт несохранения лептонного заряда и нейтринных осциляций, что является следствием наличия у нейтрино массы.

10.

53. $\left(m_{\mathrm{W}}c^2\right)_{\min} = (1+\sqrt{2}/2)\mathscr{E} \simeq 100$ ГэВ. (Современное значение $m_{\mathrm{W}}c^2 = 80,22 \pm 0,26$ ГэВ.)

10.

54. Электрон - продукт распада $\tau^- \to \mathrm{e}^- + \tilde{v}_\mathrm{e} + v_\mathrm{t}$. Искомая проекция электрона максимальна, когда $\mathbf{p}_{v_\mathrm{e}} = \mathbf{p}_{v_\mathrm{t}}$ и когда она перпендикулярна $\mathbf{p}_\mathrm{r}$. Тогда $p_\mathrm{e} \perp c = m_\tau c^2/2 = 0,896$ ГэВ.

10.

55. $m_{\boldsymbol{Z}}c^2 \approx 2p_\mu c\sin(\theta/2) = 97,5$ ГэВ; $\beta = \cos(\theta/2) = 0,82$ (Современное значение $m_Z c^2 = 91,173 \pm 0,020$).

10.

56. Минимальная длина волны γ-кванта соответствует максимальной энергии. Как видно из графика, максимальная зарегистрированная энергия (γ-квант $+\psi$) составляет 3,14 ГэВ.
$\lambda_\gamma = \frac{2\pi\hbar c}{\mathscr{E}_\gamma}$; $\mathscr{E}_\gamma = \mathscr{E}_{\max} - m_\psi c^2 = 40\mathrm{M} \ll 3,1$ ГэВ; $\lambda_\gamma \approx 3,1 \cdot 10^{-12}$ cm (пренебрегаем отдачей ψ-мезона).

10.

57* Спин мюона направлен против его импульса; $l \approx 1470$ м.

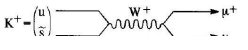
Решение. Определение спина как собственного момента импульса, т. е. момента импульса в системе покоя частицы, оказывается неприменимым к безмассовым частицам, обладающим нулевой энергией покоя, т. е. $m = 0$. Для них принято вводить спиральность, т. е. проекцию собственного момента импульса на направление движения частицы - единственное выделенное направление для частиц с $m = 0$. При этом частицы с $\mathbf{S} \uparrow\uparrow \mathbf{p}$ называются

правоспиральныцми (правополяризованными), а частицы с $\mathbf{S} \uparrow\downarrow \mathbf{p}$ называются левоспиральными (левополяризованными). При этом фотон как истинно нейтральная частица может менять свою спиральность (с номощью пластинки $\lambda/2$), а нейтрино - нет. Нейтрино но определению - левоспиральная частица, а антинейтрино - правоспиральная.

Так как каон K^+имеет спин $S = 0$, то $\mathbf{S}_\mu + \mathbf{S}_v = 0$. Кроме того, $\mathbf{p}_\mu + \mathbf{p}_\nu = 0$. Отсюда следует, что $\mathbf{S}_\mu$ антипараллелен $\mathbf{p}_\mu$ ($\mathbf{S}_\mu \uparrow\downarrow \mathbf{p}_\mu$). Для ответа на второй вопрос задачи. Запишем закон сохранения энергии при распаде

$$m_{\mathrm{K}}c^2 = \mathscr{E}_\nu + \mathscr{E}_\mu = pc + \sqrt{\left(m_\mu c^2\right)^2 + p^2c^2}, \text{ где } p_\mu = p_\nu = p.$$

Возведя это равенство в квадрат, получим



$$pc = \frac{(m_{\mathrm{K}}c^2)^2 - (m_u c^2)^2}{2m_{\mathrm{K}}c^2} = 235,6 \text{ МэВ}.$$

Полная энергия мюона

Рис. 185

$$\mathscr{E}_\mu = \sqrt{p^2c^2 + m_\mu^2 c^4} \approx 258\text{М} \ni \text{ В}.$$

Из релятивистской формулы $\mathscr{E}_\mu = m_\mu c^2/\sqrt{1-\beta^2} = \gamma m_\mu c^2$ определим: $\gamma \approx 2,444$ и $\beta = 0,912$ (относительная скорость мюона). Пробег мюона в лабораторной системе отсчета

$$l = \beta c \mathrm{r}_0 \gamma = 1,47 \cdot 10^5 \text{ cm} = 1,47\text{Km}.$$

При этом использовались табличные данные $m_\text{K}\mathrm{c}^2 = 493,6\text{М Э}$; $m_\mu c^2 = 105,7\text{М}$; $\mathbf{I}_\mu = \boldsymbol{\tau}_0 = 2,2$ мкс. Схема распада приведена на рис. 185.

10.

58. $\frac{q^2}{\hbar c} \sim \frac{\hbar}{2m_\text{n} c R_\text{d}} \sim 0,1.$

10.

59: $r_{\text{J}/\psi} = \frac{\sqrt{3}}{2} \frac{\hbar c}{\sqrt{(4\mathscr{Q}_2 - \mathscr{E}_1)(\mathscr{C}_2 - 1)}} = 1,5 \cdot 10^{-14}$ cm.

Решение. Связанная система кварк-антикварк (в данном случае (cc)) с потенциалом взаимодействия $U = -q^2/r$ аналогична позитронию и спектр ее возбуждений подобен энергетическому спектру атома водорода. Поэтому можно записать, что массы мезонов складываются из энергий покоя кварков за вычетом их энергии связи

$$\mathscr{E}_1 = 2m_c c^2 - \frac{\mu q^4}{2\hbar^2}\frac{1}{1^2}$$
$$\mathscr{E}_2 = 2m_c c^2 - \frac{\mu q^4}{2\hbar^2}\frac{1}{2^2},$$

где $\mu = m_\text{c}/2$ - приведенная масса. Здесь m_c обозначает массу с-кварка. Отличие в энергиях покоя двух состояний чармония (т. е. J/-мезона и ψ'-мезона) $\Delta\mathscr{E} = \mathscr{E}_2 - \mathscr{E}_1 = \frac{3}{16}\frac{m_c q^4}{\hbar^2}$. Из двух уравнений находим

$$m_c c^2 = \frac{4\mathscr{E}_2 - \varepsilon_\text{I}}{6} = 1,95\Gamma_\jmath\mathbf{B}$$

и характерный радиус чармония

$$r_{\text{J}/\psi} = \frac{\hbar^2}{\mu q^2} = \frac{3}{\sqrt{2}} \frac{\hbar c}{\sqrt{(4\mathscr{E}_2 - \mathscr{E}_1)(\mathscr{E}_2 - \mathscr{E}_1)}} = 1,5 \cdot 10^{-14} \text{ cm}$$

Поскольку кварки отсутствуют в свободном состоянии, то определение их энергии невозможно. Это связано с тем, что в адронах кварки окружены глюонами и виртуальными парами кварк-антикварк, и масса кварка дложна зависеть от расстояния, на котором она определяется. На расстояниях $x \lesssim 10^{-14}$ см, где начинается асимптотическая свобода и «облака» глюонов и виртуальных кварковых пар «редеют», принято говорить о токовых (свободных) кварках. На больших расстояниях мы имеем дело с «одетыми» кварками, которые называются блоковыми или конституентными. (см. Приложение III, табл. 5).

В рамках данного приближения по результатам эксперимента можно определить, как энергию покоя кварков, так и энергию их взаимодействия.

10.

60. $m_\text{B}c^2 = \frac{1}{6}(4\mathscr{E}_2 - \mathscr{E}_1) \approx 5,1\Gamma \ni \text{ В}; g^4 = \left(\frac{q^2}{\hbar c}\right)^2 = 32\frac{(\mathscr{E}_2 - \mathscr{E}_1)}{(4\mathscr{E}_2 - \mathscr{E}_1)} \approx 0,585,\ g^2 \approx 0,765 \sim 1.$

10.

61. $R \approx \frac{\hbar c}{m_\text{W} c^2} \approx 2,5 \cdot 10^{-16}$ cm.

10.

62. $m_\Delta c^2 = \sqrt{2m_\text{p}c^2T_\pi + (m_\text{p}+m_\pi)^2c^4} = 1232,5\text{МЭ}$;
$\tau \approx \frac{\hbar}{\Gamma} = 5,5\cdot 10^{-24}\text{с}$.

10.

63*. Решение. Резонансный характер поглощения пионов свидетельствует об образовании составного ядра, которое можно уподобить короткоживущей частице. Сечение образования составного ядра в резонансной области (рис. 186) определяется для бесспиновых частиц формулой Брейта-Вигнера

$$\sigma_\text{полн} = \pi\lambda^2\frac{\Gamma_\text{упр}\,\Gamma_\text{полн}}{(\mathscr{E}-\mathscr{E}_0)^2+\frac{\Gamma^2_\text{полн}}{4}},$$

где $\lambda = \frac{\lambda}{2\pi}, \lambda$ - длина волны падающей частицы в системе центра масс, $\mathscr{E}$ - суммарная энергия частиц в этой системе, $\mathscr{E}_0$ - энергия составного ядра (резонанса), $\Gamma_{\text{упр и}}$

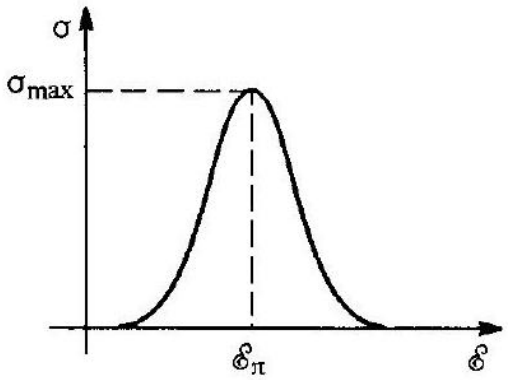


Рис. 186 $\Gamma_\text{неупр} = \Gamma_\text{полн} - \Gamma_\text{упр}$ - ширины резонанса, связанные с распадом по упругому и неупругим каналам.

Согласно закону сохранения электрического заряда распад резонанса возможен только по каналу $\Delta \to \pi^+ p$, то есть происходит только упругое рассеяние и в резонансе сечение

$$\sigma_\text{полн} = \sigma_\text{упр} = 4\pi t^2 = \frac{4\pi\hbar^2}{p^2}$$

Импульс сталкивающихся частиц в системе центра масс $p = p_\pi = p_\text{p}$ находитея из условия

$$M_\Delta c^2 = \sqrt{(pc)^2 + (m_\text{p}c^2)^2} + \sqrt{(pc^2) + (m_\pi c^2)^2}$$

откуда

$$p = \sqrt{\frac{\left(M_\Delta^2 + m_\text{p}^2 - m_\pi^2\right)^2}{4M_\Delta^2}c^2 - m_\text{p}^2c^2} = 227\text{МэВ}/c;$$

$$\sigma_\text{полн} = \frac{4\pi\hbar^2c^2}{p^2c^2} = 95\cdot 10^{-27}\ \text{см}^2 = 95\ \text{м б}\ .$$

Экспериментальное значение для данной реакции $\sigma_\text{полн} \simeq 200$ мбн. Различие связано с тем, что в простейшем варианте формулы Брейта-Вигнера не учитываются спиновые состояния начального и конечного состоя ния системы. Имеются $(2S_\text{p}+1)(2S_\pi+1)$ начальных состояний системы и $2J+1$ конечных состояний Δ-резонанса, приводящих к одинаковому сечению.

В результате в формуле Брейта-Вигнера появляется множитель $g = \frac{2J+1}{(2S_\text{p}+1)(2S_\pi+1)}$, учитывающий стастистический вес входного и выходного состояний системы. Сравнение теоретического и экспериментальных значений позволяет определить, что $g \simeq 2$, откуда находится полный момент резонанса $J = 3/2$.

Полученный результат требует пояснения. Так как $S_\text{p} = 1/2; S_\pi = 0$, то в сумме они не могут дать $J = 3/2$. Поэтому необходимо учитывать и орбитальное движение, т. е. закон сохранения момента нужно записывать в виде $\mathbf{J} = \mathbf{S}_\text{p} + \mathbf{S}_\pi + \mathbf{L}_\pi$, где $\mathbf{L}_{\pi\text{p}}$ - орбитальный момент относительного движения. Считая, что радиус протона $r_\text{p} \simeq 0,8\cdot 10^{-13}$ см (фактически это комптоновская длина волны протона), получаем $pr_\text{p} = \hbar\sqrt{L(L+1)}$, или $\sqrt{L(L+1)} = \frac{r_\text{p}}{\hbar}$. Так как $\lambda = 0,87\cdot 10^{-13}$с, то $L \simeq 0,83$. Следовательно, возможные значения $L = 0,1$. Соображения, основанные на законе сохранения четности, показывают, что $L = 1$ и $J = 1/2 + 1 = 3/2$. Образно говоря, пролетающий пион захватывается за счет сильного взаимодействия протоном на орбиту с $L = 1$, делает несколько оборотов и затем улетает.

Во второй реакции (в отличие от предыдущей) возможен распад резонанса

$$\pi^- + p \to \Delta^0 \to \left\{ \begin{array}{l} \pi^- + p \\ \pi^0 + n \end{array} \right.$$

и таким образом появляется «неупругий» канал.

$$\sigma_{\text{полн}} = \sigma_{\text{упр}} + \sigma_{\text{неупр}} ,$$

где в резонансе

$$\sigma_{\text{полн}} = 8\pi\pi^2 \frac{\Gamma_{\text{упр}}}{\Gamma_{\text{полн}}} \quad \text{или} \quad 68 \approx 190 \frac{\Gamma_{\text{упр}}}{\Gamma_{\text{полн}}},$$

откуда
$\frac{\Gamma_{\text{упр}}}{\Gamma_{\text{полн}}} = \frac{\sigma_{\text{упр}}}{\sigma_{\text{упр}} + \sigma_{\text{неупр}}} \approx 0,358; \quad \sigma_{\text{неупр}} \approx 1,8\sigma_{\text{упр}} \approx 0,64\sigma_{\text{полн}} \approx 44$ мбн.
Отметим, что другие неупругие процессы типа $\pi^0\pi^0 n$ или $\pi^-\pi^0$p запрещены законами сохранения энергии.

Рассмотренные резонансные состояния Δ^{++}и Δ^0 различаются проекциями изотопического спина. Изотопический спин пионов 1 , а нуклонов 1/2. Полный изоспин резонанса поэтому может быть 3/2 и 1/2. При этом (π^+p) система обладает проекцией изоспина $T_3 = 3/2$, а ($\pi^- p$) - проекцией $T_3 = 1/2$, т. е. является суперпозицией состояний с $T = 3/2$ и $T = 1/2$.

10.

64. p = (uud); n = (udd) ; Ω^- = (sss).

10.

65. $\pi^+ = (ud); K^+ = (u\tilde{s})$.

10.

66. $\mathrm{K}^0 = (\mathrm{d}\tilde{\mathrm{s}}), \tilde{\mathrm{K}}^0 = (\tilde{\mathrm{d}})$.

10.

67. Ξ^0 = (uss) ; Λ = (uds).

10.

68. $\pi^-; K^-$.

10.

69* $\sigma_3 = 2\sigma_2 - \sigma_1$.
Решение. Кварковый состав частиц из задачи:

$$\mathrm{K}^+ = (\mathrm{us}), \quad \Sigma^+ = (\mathrm{uus}\ ), \quad \Xi^0 = (\ \mathrm{uss}\ ), \quad \Omega^- = (\mathrm{sss})$$

Обозначим сечения взаимодействия кварков, имея в виду, что в задаче могут взаимодействовать кварки двух поколений: и - из первого поколения, s - из второго. Кроме того, заметим, что при $\mathscr{E} \gg c^2$ сечения рассеяния частицы и античастицы одинаковы (теорема Померанчука). Таким образом,

$$\begin{array}{l} \sigma_a = \sigma(\mathrm{uu}) \approx \sigma(\mathrm{ud}) = \sigma(\mathrm{u}\ \tilde{\mathrm{d}}) = \sigma(\tilde{\mathrm{u}}\ \tilde{\mathrm{d}}) \\ \sigma_b = \sigma(\mathrm{us}) = \sigma(\mathrm{us}) \approx \sigma(\mathrm{d}\ \tilde{\mathrm{s}}) = \sigma(\tilde{\mathrm{u}}s) \text{ и т. д.;} \\ \sigma_c = \sigma(\mathrm{ss}) = \sigma(\mathrm{s}\ \tilde{\mathrm{s}}) = \sigma(\tilde{\mathrm{s}}s) \end{array}$$

Рассмотрим в качестве примера первую реакцию (рис. 187). Стрелками обозначены взаимодействия кварков: сплошная стрелка - с сечением σ_a; штриховая стрелка - с сечением σ_b; волнистая стрелка - с сечением σ_c. При указанных в задаче энергиях дебройлевская длина волны кварков оказывается много меньше размера частиц. Поэтому можно считать, что происходят

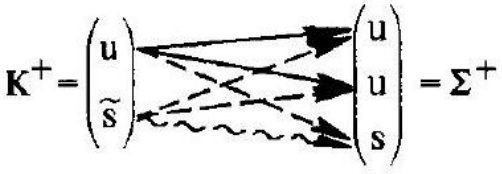


Рис. 187 только одночастичные взаимодействия кварков и в каждой из указанных реакций сечения надо просуммировать по всем возможным каналам. Таким образом, сечение взаимодействия

$$\sigma_1 = 2\sigma_a + 3\sigma_b + \sigma_c$$

Вторая реакция $\mathrm{K}^+ + \Xi^0$ дает сечение

$$\sigma_2 = \sigma_a + 3\sigma_b + 2\sigma_c$$

Аналогичное рассмотрение взаимодействия $\mathrm{K}^+ + \Omega^-$приводит к следующему выражению

$$\sigma_3 = 3\sigma_b + 3\sigma_c.$$

Решая полученную систему уравнений, выражаем неизвестное сечение σ_3 через заданные сечения σ_1 и σ_2:

$$\alpha_3 = 2\alpha_2 - \sigma_1.$$

10.

70. $\sigma(\pi\mathrm{p}) = 26$ мбн, $\sigma(\Lambda N) = 32$ мбн; $\sigma(\Xi N) = 25$ мбн.

10.

71. $\alpha(\Lambda N) = 32$ мбн; $\sigma(EN) = 25$ мбн, $\sigma(\Omega N) = 18$ мбн.

10.

72. $m_\Xi \approx m_\mathrm{u} + 2m_\mathrm{s} \approx m_\mathrm{u} + 2\,(\Delta + m_\mathrm{u}) \approx 1290\mathrm{M} \ni \mathrm{B}$.
Замечание. Речь идет о блоковых (тяжелых) кварках, и $m_\mathrm{d} \approx m_\mathrm{u}$. Поэтому $m_\Lambda - m_\mathrm{p} = m_\mathrm{s} - m_\mathrm{u}$.

10.

73. а) $v_\mu + p \to \mu^- + \Delta^{++}$. Здесь возможны две схемы реакции (рис. 188):
б) $\nu_\mu + \mathrm{n} \to \mu^- + \mathrm{p}$ или $\mu^- + \Delta^+$;
в) $\tilde{v}_\mu + \mathrm{p} \to \mu^+ + \mathrm{n}$ или $\mu^+ + \Delta^0$;
г) $\tilde{\nu}_\mu + n \to \mu^+ + \Delta^-$.

Рис. 188
Отношение эффективных сечений этих реакций $\sigma_a : \sigma_\sigma : \sigma_6 : \sigma_2 = 1 : 2 : 2 : 1$.

10.

74. Решение. Схема распада протона $\mathrm{p} \to \pi^0 + \mathrm{e}^+$изображена на рис. 189. Масса X -бозона определяется из соотношения неопределенностей

$$Mc^2 \approx \frac{\hbar}{\tau} \approx 0,6 \cdot 10^{23} \ni \text{ B} = 0,6 \cdot 10^{14}\Gamma \ni \text{ B}.$$

Заряд X-бозона равен сумме зарядов двух и-кварков

$$Q_X = +\frac{4}{3}e$$

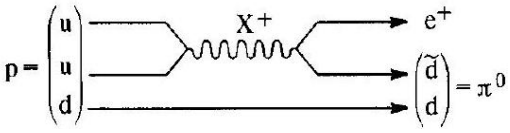


Рис. 189

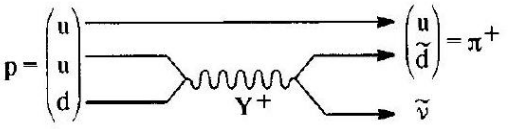


Рис. 190

10.

75. $R \approx 2 \cdot 10^{-29}$ cm; $Q_Y = +e/3$. Схема распада изображена на рис. 190.

10.

76: Решение. На рис. 191 и 192 показаны все $24(2 \times 12)$ перехода между кварками и лептонами, идущих через нейтральный Z^0 и заряженные

промежуточные бозоны $\mathrm{W}^{\pm}$, допустимые по теории электрослабого взаимодействия. При этом не наблюдавшиеся экспериментально переходы $t \leftrightarrow s$ и $t \leftrightarrow d$ изображены штриховыми линиями. Приведем примеры наблюдаемых переходов:

$$\mathrm{e}^+ + \mathrm{e}^- \to \mathrm{Z}^0 \to v_l + \tilde{v}_l, \text{ где } l \equiv \mathrm{e}, v, \tau - \text{ лептоны},$$

- это рождение нейтринных пар в результате ее-столкновений;

$$\mathrm{e}^+ + \mathrm{e}^- \leftrightarrow \mathrm{Z}^0 \leftrightarrow \mathrm{u} + \tilde{\mathrm{u}}$$

- рождение в ее-столкновениях и распад в адроны, либо рождение в р рстолкновениях и распад на пару лептон-антилептон;

$$\mathrm{d} \to \mathrm{u} + \mathrm{w}^- \to \mathrm{u} + \mathrm{e}^- + \tilde{v}_{\mathrm{e}}$$

- распад нейтрона;

$$\mathrm{u} + \tilde{\mathrm{d}} \to \ \mathrm{W}^+ \to \tilde{l} + v_l, \text{ где } l \equiv \mathrm{e}, \mu, \mathrm{r} \text{ - лептоны}$$

- рождение в р $\tilde{p}$-столкновениях и распад на пару лептон-антилептон.

Как следует из рис. 191 в процессах с участием Z^0-бозона аромат кварков не меняется. На рис. 193 приведены доминирующие при слабых распадах адронов переходы между кварками, идущие через обмен $W^{\pm}$-бозонами. В то же время допустимые законом сохранения заряда переходы $c \to d$, $b \to u$ и другие, изображенные на рис. 192, так же возможны. Например, экспериментально наблюдается как распад $D^0 \to K^- + \pi^+$, соответствующий переходу $c \to \tilde{s}$ (рис. 194), так и распад $D^0 \to \pi^- + \pi^+$, соответствующий переходу $c \to d$. Отношение вероятностей этих переходов составляет $5 \cdot 10^{-2}$. Переходы же через поколение подавлены еще сильнее.

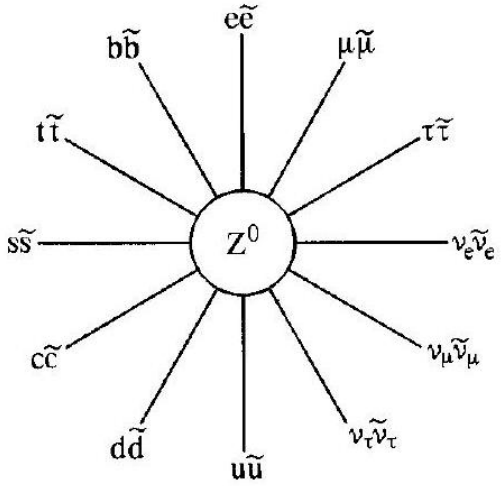


Рис. 191

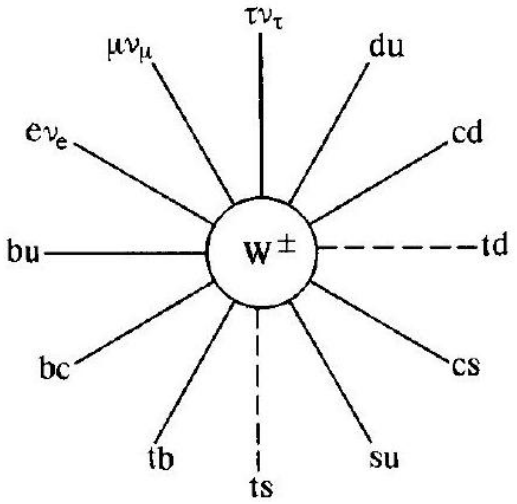


Рис. 192

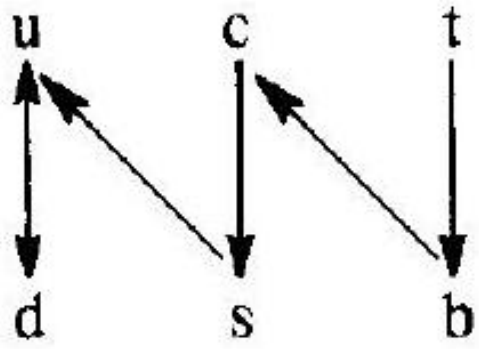


Рис. 193

В условии задачи B^--мезон, имеющий кварковый состав (b), в вершине 2 (рис. 64 из условия) распадается. Наиболее вероятный процесс - это распад b кварка по схеме $b \to c + W^-$(преобразование в ближайший более легкий кварк второго поколения).

Таким образом, в вершине 2 рождается тяжелая частица с кварковым составом (си). Это D^0-мезон, т. е. $X \equiv D^0$. Кроме того, в эмульсии оставил

след возможно мюон, поскольку образовавпийся при распаде b -кварка W^-бозон мог распасться по схеме

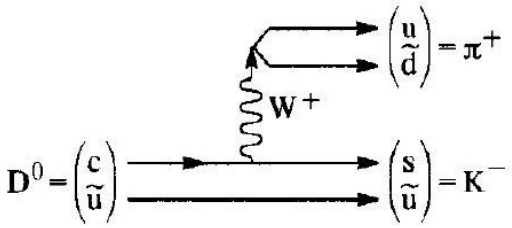


Рис. 194

$$W^- \to \left\{ \begin{array}{l} \mu^- + \tilde{\upsilon_\mu} \\ \mathrm{e}^- + \tilde{\upsilon_\mathrm{e}} \\ \tau^- + \tilde{\upsilon_\tau} \end{array} \right.$$

Далее в вершине $3\mathrm{D}^0$-мезон распадается. Схема его распада изображена на рис. 194. Наиболее вероятен распад скварка в рамках второго поколения по схеме

$$\mathrm{c} \to \ \mathrm{s} + \mathrm{W}^+$$

В свою очередь W^+-бозон распадается, как сказано в условии задачи, по нелептонному каналу. Наиболее вероятен такой распад:

$$\mathrm{W}^+ \to \mathrm{u} + \tilde{\mathrm{d}} \equiv \pi^+.$$

Таким образом, в вершине $3\mathrm{D}^0$-мезон распадается по схеме:

$$\mathrm{D}^0 \to \ \mathrm{K}^- + \pi^+, \quad \text{где} \quad \mathrm{K}^- = (\mathrm{s}\tilde{\mathbf{u}})$$

Возможны и другие каналы распада D^0-мезона через K^--мезон с образованием любого числа пионов: $\mathrm{D}^0 \to \ \mathrm{K}^- + \pi^+\pi^0$ или, например, $\mathrm{D}^0 \to \ \mathrm{K}^- + \pi^+ + \pi^+ + \pi^-$.

10.

77. Неизвестная частица X - это Ω^--гиперон. При соударении K^-и p кроме Ω^-образовались еще две частицы. Это пара каонов K^0 и K^+.

10.

78: Странность частицы $S = 1$. Это могут быть K^0, а также D^0, или B^0.

Решение. По условию задачи электрический и барионный заряды частицы равны $Q = 0, B = 0$, а проекция изотопического спина $T_3 = -1/2$. Ответ надо искать, очевидно, среди мезонов, т.е. частиц, имеющих состав (кварк, антикварк).

По условию это может быть странный мезон, хотя не исключен очарованный или красивый мезон. Воспользуемся формулой Гелл-Мана-Нишиджимы

$$Q = T_3 + \frac{1}{2}(B + S + C + b + t) = T_3 + \frac{1}{2}Y$$

где B - барионный заряд, S - странность, C - очарование, b - красота, t - правдивость, Y - гиперзаряд. Подстановка в эту формулу данных задачи дает уравнение (для случая поиска странного мезона)

$$0 = -\frac{1}{2} + \frac{1}{2}(0 + S)$$

откуда $S = 1$. Таким образом, это $\mathrm{K}^0 = (\mathrm{d}\tilde{\mathrm{s}})$. В принципе, это может быть и очарованный мезон $\mathrm{D}^0 = (\tilde{\mathbf{u}})$. В этом случае по формуле Гелл-Мана - Нишиджимы должно быть $C = 1$. Также не исключен случай совсем редкой частицы с кварками третьего поколения B^0-мезон.

10.

79. Антинейтрон n.

10.

80. $Y = -2, S = -3.\Omega^-$-гиперон.

10.

81. $Y = -1; S = -2.\Xi^0 \equiv$ (uss)-гиперон.

10.

82. $\mu_{\Delta^{++}} = 2\mu_{\text{p}} = 5,6\mu_{\text{гд}}$.

10.

83. $\mu_{\Omega^-} = 1,7\mu_{\text{яд}}$. Масса странного кварка принята равной $m_{\text{s}} \approx \approx M_\Omega/3 \approx 557\text{M} \ni \text{B}$.

10.

84* $k \approx 8 \cdot 10^{27}$ монополей.

Решение. Монополь, летящий со скоростью $v = \sqrt{2\text{Å}/M}$, в 1 с инициирует $N =$ опи распадов протонов (σ - сечение реакции, n - концентрация протонов). При этом освобождается энергия

$$Nm_{\text{p}}c^2 = \sigma nvm_{\text{p}}c^2$$

переходящая в тепло при поглощении позитрона и γ-квантов. По условию $k\sigma nvm_{\text{p}}c^2 = L_{\text{C}}$, где k - число монополей в Солнце. Сечение реакции распада протона находится из условия распада одного протона на длине 1c : $n_{\text{p}}\alpha = 1$; $\sigma = 1/n_{\text{p}} = 3 \cdot 10^{-24}$ cm^2, где n_{p} - концентрация протонов в 1 cm^3 воды, $n_{\text{p}} = 10N_{\text{A}}(\text{m}/\mu) \approx 3,3 \cdot 10^{23}$ cm^{-3}, (в молекуле воды 10 протонов).

Число протонов в 1 cm^3 Солнца

Отсюда

$$n = \frac{\rho}{m_{\text{p}}} = \frac{M_{\text{C}}}{(4/3)\pi R_{\text{C}}^3}\frac{1}{m_{\text{p}}}$$

$$k = \frac{L_{\text{C}}}{\sigma nvm_{\text{p}}c^2} = \frac{4L_{\text{C}}n_{\text{p}}\pi R_{\text{C}}^3}{3M_{\text{C}}c^2\sqrt{2\mathscr{E}/M}} \approx 8 \cdot 10^{27}$$

10.

85* $\mathscr{E}_{\text{пор}} \approx 270$ ГэВ.

Решение. На встречных пучках протонов (uud) и антипротонов () может родиться реальный W^+_- $\text{u} + \tilde{\text{d}} = \text{W}^+$, если $\mathscr{E}_{\text{W}} > m_{\text{W}}c^2$. В ультрарелятивистском случае энергия распределяется между кварками точно так же, как и импульс. По закону сохранения энергии

Откуда

$$\mathscr{E}_{\text{пор}} = \frac{m_{\text{W}}c^2}{0,3} \approx 270 \text{ ГэВ}$$

Совершенно аналогично при столкновении кварков d и и может родиться W^--бозон. Порог реакции будет таким же.

10.

86. $_{\text{пор}} \approx 300$ ГэВ.

10.

87. См. рис. 195.

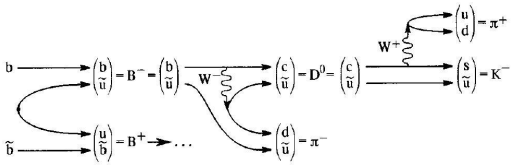


Рис. 195

10.

88. См. рис. 196.

10.

89. См. рис. 197.

10.

90. См. рис. 198.

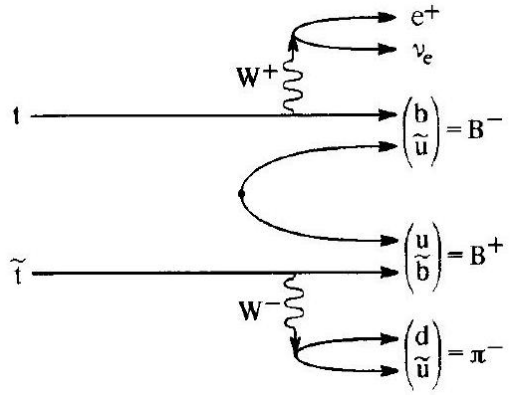


Рис. 196

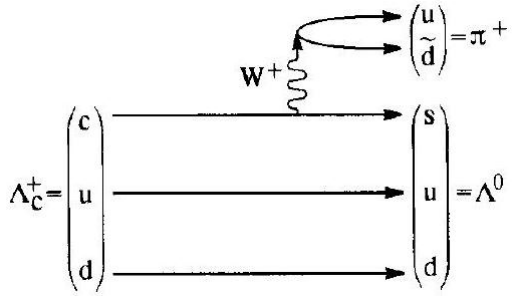


Рис. 197

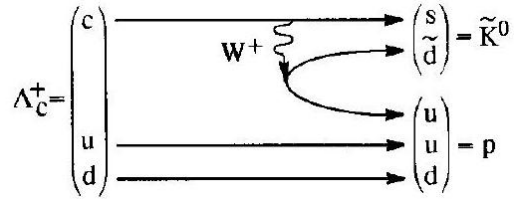


Рис. 198

10.

91. Заметим, что реакция $v_{\mathrm{e}} + \mathrm{p} \rightarrow \mathrm{n} + \mathrm{e}^{+}$не идет, поскольку запрещена законом сохранения лептонного заряда. Поэтому реакция может идти только на нейтронах. Причем, так как энергия нейтрино меньше 15 М МВ, то возможно детектирование только электронных нейтрино v_{e} на нейтронах дейтерия в реакции $v_{\mathrm{e}} + {}^{2}_{1}\,\mathrm{d} \rightarrow \mathrm{p} + \mathrm{p} + \mathrm{e}^{-}$, откуда $\mathscr{E}_{\text{пор}} = 1,37\text{М эВ}$.

10.

92. $\mathscr{E}^{\Pi\circ\rho}_{\nu_e} = 15,5\text{М }\ni;\ ;\mathscr{E}^{\Pi\circ}_{\gamma_\mu} = 121,5\text{М ВВ}$.

10.

93*: $\frac{\mu_{\mathrm{n}}}{\mu_{\mathrm{p}}} = -\frac{2}{3} = -0,667$ (эк сперимент дает $\frac{\mu_{\mathrm{n}}}{\mu_{\mathrm{p}}} = -0,685$).

Решение. Для протона вероятность спинового состояния ($\uparrow \mathbf{u}, \uparrow u, \downarrow\ \mathrm{d}$) равняется 2/3, а спинового состояния ($\uparrow \mathrm{u}, \downarrow \mathrm{u}, \uparrow \mathrm{d}$) равняется 1/3 (согласно условию). Следовательно, предполагая, что магнитный момент кварка пропорционален его заряду, получим, что $\mu_u = \frac{2}{3}\mu_1$; $\mu_{\mathrm{d}} = -\frac{1}{3}\mu_1$, где μ_1 - «элементарный» магнитный момент. Таким образом, магнитный момент протона равен

$$\mu_p = \frac{1}{3}\left(\frac{2}{3}\mu_1 - \frac{2}{3}\mu_1 - \frac{1}{3}\mu_1\right) + \frac{2}{3}\left[\frac{2}{3}\mu_1 + \frac{2}{3}\mu_1 - \left(-\frac{1}{3}\mu_1\right)\right] = 3\mu_1$$

Аналогично для нейтрона состояние ($\uparrow \mathrm{d}, \uparrow \mathrm{d}, \downarrow \mathrm{u}$) имеет вероятность 2/3, а состояние ($\uparrow \mathbf{d}, \downarrow \mathbf{d}, \uparrow \mathbf{u}$) - вероятность 1/3. Поэтому

$$\mu_{\Pi} = \frac{2}{3}\left(-\frac{1}{3}\mu_I - \frac{1}{3}\mu_1 - \frac{2}{3}\mu_1\right) + \frac{1}{3}\left[-\frac{1}{3}\mu_1 - \left(-\frac{1}{3}\mu_1\right) + \frac{2}{3}\mu_1\right] = -2\mu_1$$

Откуда искомое отношение $\frac{\mu_{\mathrm{n}}}{\mu_{\mathrm{p}}} = -\frac{2}{3} = -0,667$, тогда как экспериментальное значение $\left(\frac{\mu_n}{\mu_p}\right)_{\text{эксп}} = -0,685$.

Покажем, почему появляются вероятности 1/3 и 2/3 при разных спиновых состояниях протона. Каждый кварк имеет спин 1/2, поэтому максимальный спин системы из трех кварков равен 3/2 - это состояние ($\uparrow \mathrm{u}, \uparrow \mathrm{u}, \uparrow \mathrm{d}$), соответствующее Δ^{+}-изобаре.

Если перевернуть спин одного из кварков в Δ^{+}-изобаре, то получим систему со спином 1/2. Таких состояний возможно три: ($\uparrow \mathbf{u}, \uparrow u, \downarrow d$), ($\uparrow \mathrm{u}, \downarrow \mathrm{u}, \uparrow \mathrm{d}$) и ($\downarrow \mathrm{u}, \uparrow \mathrm{u}, \uparrow \mathrm{d}$). При этом последние два совершенно неразличимы физически - это одно состояние. Таким образом, вероятность состояния ($\uparrow u, \uparrow u, \downarrow d$) вдвое выше состояния ($\uparrow u, \downarrow u, \uparrow d$) и составляет 2/3 против 1/3 в последнем случае.

Аналогично можно поступить и в системе кварков, ($\uparrow\ u, \uparrow\ d, \uparrow\ d$), соответствующей Δ^{0}-изобаре, имеющей спин 3/2. Если перевернув спин одного из кварков, получить систему со спином 1/2, то таких вариантов также три: ($\downarrow \mathrm{u}, \uparrow \mathrm{d}, \uparrow \mathrm{d}$), ($\uparrow \mathrm{u}, \downarrow \mathrm{d}, \uparrow \mathrm{d}$) и ($\uparrow \mathrm{u}, \uparrow \mathrm{d}, \downarrow \mathrm{d}$). Последние два варианта физически неотличимы. Поэтому вероятность состояния ($\downarrow \mathrm{u}, \uparrow \mathrm{d}, \uparrow \mathrm{d}$) вдвое больше состояния ($\uparrow \mathrm{u}, \downarrow \mathrm{d}, \uparrow \mathrm{d}$) и составляет 2/3 против 1/3.

Заметим, что разность масс Δ-изобар и нуклонов связана только с переворотом спина, а не с возникновением орбитального момента кварка. И нуклон и Δ-изобары - это S-состояния с различными $J: 1/2$ и $3/2$.

Сейчас к проблеме магнитных моментов нуклонов развит более наглядный подход, основанный на обобщенном принципе Паули. Согласно этому принципу волновая функция нуклона (произведение орбитальной, спиновой, изоспиновой и цветовой функций кварков) должна быть антисимметрична относительно перестановки любой пары тождественных кварков. Отсюда следует, что спины одинаковых кварков в нуклонах параллельны (цветовая функция всегда антисимметрична, орбитальная функция при $l = 0$ симметрична, следовательно изоспиновая и спиновая функции - симметричны). Тем самым задача вычисления магнитных моментов нуклонов сводится к вычислению суммарного магнитного момента двух частиц со спином 1 (пара одинаковых кварков с параллельными спинами) и одной со спином 1/2 (оставшийся кварк).

10.

94. $\mathscr{E} = (m_\Delta - m_n)\,c^2 = 1231 - 939 = 292\text{М ЭВ}$. (См. решение задачи

10.

93.)

10.

95. $\tau \simeq \frac{\hbar}{\alpha^2 m_e c^2} \frac{8 r_{\text{Б}}^3}{\text{Å}_e^3} = \frac{8 r_{\text{кл}}}{\alpha^6 c} = 5 \cdot 10^{-10} c$, где $r_{\text{Б}}$ - боровский радиус электрона в атоме водорода, $r_{\text{кл}} = \frac{e^2}{mc^2}$ - классический радиус электрона.

10.

96. $t_{\text{р}} \simeq t_{\text{яд}} \frac{r_{1\text{p}}^3}{\text{Å}_\pi^3} = 0,32 \cdot 10^{-18}$с, где $\text{А} = \frac{\hbar}{m_\pi c} = 1,4 \cdot 10^{-13}$с - комптоновская длина волны пиона (радиус сильного взаимодействия), $t_{\text{яд}} \simeq 0,5 \cdot 10^{-23}$ с - характерное «ядерное время», r_{1p} - радиус основного состояния протониума.

10.

97* $\mathscr{E}_{\Gamma\pi} = \frac{m_{\text{n}} c^2}{4}; R_{\text{П}} = \frac{4\pi\hbar}{m_{\text{n}} c} = 2,64$ фм.

Решение. Волновая функция основного сферически симметричного состояния (орбитальный момент равен нулю) частицы в трехмерной сферической яме с непроницаемыми стенками $\psi = A\frac{\sin kr}{r}$. Условие на границе $\psi(R) = 0$ дает разрешенные значения волновых чисел $k = \frac{\pi}{R} n$. Таким образом, минимальная энергия трех безмассовых кварков в непроницаемой сфере $\mathscr{E}_{\text{Кв}} = 3\hbar kc = \frac{3\pi\hbar c}{R}$, т. к. из-за различия в цвете они могут втроем находится на нижнем уровне. Обозначим плотность энергии глюонного поля через ε. Тогда энергия кварков и глюонов

$$\mathscr{E} = \mathscr{E}_{\text{КВ}} + \mathscr{E}_{\text{ГЛ}} = \frac{3\pi\hbar c}{R} + \varepsilon \frac{4}{3}\pi R^3$$

Минимизируя это выражение, получаем

$$R_{\min} = \left(\frac{3\hbar c}{4\varepsilon}\right)^{1/4}, \text{ а } \mathcal{E}_{\min} = 4\pi\hbar c \left(\frac{4\varepsilon}{3\hbar c}\right)^{1/4} = \frac{4\pi\hbar c}{R_{\min}}$$

Поскольку $\mathscr{E}_{\min} = m_{\text{n}} c^2$, то

$$R_{\text{n}} = R_{\min} = 4\pi \frac{\hbar}{m_{\text{n}}} = 4\pi t_{\text{n}} = 2\lambda_{\text{n}} = 2 \cdot 1,32 \cdot 10^{-13} \phi\text{М}$$

Энергия глюонного поля составляет:

$$\mathscr{E}_{\text{г}J} = \varepsilon \cdot \frac{4}{3}\pi R_{\min}^3 = \frac{\pi\hbar c}{R_{\min}} = \frac{m_{\text{n}} c^2}{4}$$

т. е. четверть энергии покоя нуклона.

10.

98. Поскольку $\sigma(\mathscr{E}) \propto \mathscr{E}^2$, то $\frac{\sigma(\mathscr{E}=1\text{М. })}{\sigma(\mathscr{E}=10\text{М В })} = 10^{-2}$.

19 Problems about Formalism of QM

19.1 Problems about Operators

19.1.1 Problems about Basic Quantum Operators

(начало белоусова и любого типичного курса. в запись про простые задачи перенесу то, что простое и скучное.)

ПТФ-1.y1. Унитарные матрицы

Покажите, что унитарные матрицы, как и эрмитовы, диагонализуемы. *Указание*: покажите, что эрмитова и анти-эрмитова часть унитарного оператора диагонализуемы совместно.

Solution.

Разложим унитарный оператор на эрмитову и анти-эрмитову части:

$$\hat{U} = \frac{\hat{U} + \hat{U}^\dagger}{2} + i\frac{\hat{U} - \hat{U}^\dagger}{2i}$$

Вычислим их коммутатор, учитывая унитарность оператора $\hat{U}$ ($\hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = \mathbb{I}$):

$$[\hat{U} + \hat{U}^\dagger, \hat{U} - \hat{U}^\dagger] = \hat{U}\hat{U} + \hat{U}^\dagger\hat{U} - \hat{U}\hat{U}^\dagger - \hat{U}^\dagger\hat{U}^\dagger - \hat{U}\hat{U} + \hat{U}^\dagger\hat{U} - \hat{U}\hat{U}^\dagger + \hat{U}^\dagger\hat{U}^\dagger = 2(\hat{U}^\dagger\hat{U} - \hat{U}\hat{U}^\dagger) = 0$$

Часть $\frac{\hat{U}+\hat{U}^\dagger}{2}$ эрмитова, $i\frac{\hat{U}-\hat{U}^\dagger}{2i}$ антиэрмитова. Докажем следующее предложение:
Если операторы коммутируют, то их можно одновременно диагонализировать.

Proof. Пусть $\vec{a}$ – собственный вектор оператора $\hat{A}$, соответствующий некратному собственному значению λ ($\hat{A}\vec{a} = \lambda\vec{a}$). Вектор $\hat{B}\vec{a}$ тоже будет принадлежать собственному значению λ матрицы A:

$$\hat{A}\hat{B}\vec{a} = \hat{B}\hat{A}\vec{a} = \lambda\hat{B}\vec{a}$$

Следовательно, вектор $B\vec{a}$ пропорционален $\vec{a}$, т.е. $\vec{a}$ является собственным вектором матрицы $\hat{B}$.
В случае кратного собственного значения λ имеем несколько собственных векторов x_i, принадлежащим этому собственному значению. Пусть $Bx_i = b_{ij}x^j$, где b_{ij} – некоторые числа. Матрицу b_{ij} можно диагонализовать, выбрав в качестве принадлежащих λ собственных векторов матрицы $\hat{A}$ другие векторы $y_i = c_{ij}x^j : Ay_i = \lambda y_i$ и $By_i = \Lambda_i y_i$ (в последнем равенстве суммы по i нет).
Т.е. у операторов общая система собственных векторов. Можно перейти к базису, состоящему из собственных векторов, и в этом базисе обе матрицы будут диагональны. □

Таким образом, эрмитова и анти-эрмитовы части диагонализуемы совместно. Следовательно, и их сумма – унитарный оператор $\hat{U}$ диагонализуем.

ПТФ-1.y2. Замена базиса

В квантовой механике замена базиса реализуется унитарными преобразованиями $|\psi'\rangle = \hat{U}|\psi\rangle$.
• Покажите, что гамильтониан при этом заменяется на $\hat{H}' = \hat{U}\hat{H}\hat{U}^\dagger$.
• Последнее утверждение необходимо модифицировать, если унитарное преобразование зависит явно от времени $\hat{U} = \hat{U}(t)$. Покажите, что в таком случае гамильтониан необходимо заменить на $\hat{H}' = \hat{U}\hat{H}\hat{U}^\dagger - i\hbar\hat{U}\partial_t\hat{U}^\dagger$.

Solution.

Запишем нестационарное уравнение Шрёдингера:

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = \hat{H}|\psi\rangle$$

Поскольку преобразование $\hat{U}$ унитарное, то

$$\hat{U}\hat{U}^\dagger = \hat{\mathbb{I}} \to \hat{U}^{-1} = \hat{U}^\dagger \to |\psi\rangle = \hat{U}^\dagger|\psi'\rangle$$

- $$i\hbar\frac{\partial(\hat{U}^\dagger|\psi'\rangle)}{\partial t} = \hat{H}\hat{U}^\dagger|\psi'\rangle \to i\hbar\frac{\partial|\psi'\rangle}{\partial t} = \hat{U}\hat{H}\hat{U}^\dagger|\psi'\rangle$$

Таким образом,

$$\hat{H}' = \hat{U}\hat{H}\hat{U}^\dagger$$

- $$i\hbar\frac{\partial(\hat{U}^\dagger(t)|\psi'\rangle)}{\partial t} = \hat{H}\hat{U}^\dagger|\psi'\rangle \to i\hbar\hat{U}^\dagger\frac{\partial|\psi'\rangle}{\partial t} + i\hbar|\psi'\rangle\partial_t\hat{U}^\dagger = \hat{U}\hat{H}\hat{U}^\dagger|\psi'\rangle$$

$$i\hbar\frac{\partial|\psi'\rangle}{\partial t} = (\hat{U}\hat{H}\hat{U}^\dagger - i\hbar\hat{U}\partial_t\hat{U}^\dagger)|\psi'\rangle$$

$$H' = \hat{U}\hat{H}\hat{U}^\dagger - i\hbar\hat{U}\partial_t\hat{U}^\dagger$$

ПТФ-1.у3. Матрицы Паули

Покажите следующие свойства матриц Паули (по повторяющимся индексам подразумевается суммирование):

• Они, совместно с единичной матрицей $\sigma^0 = \hat{\mathbb{I}}_{2\times2}$, представляют собой базис в пространстве эрмитовых матриц 2×2.

• Они удовлетворяют следующими правилам перемножения: $\hat{\sigma}^\alpha\hat{\sigma}^\beta = \delta_{\alpha\beta}\hat{\mathbb{I}} + i\epsilon_{\alpha\beta\gamma}\hat{\sigma}^\gamma$ ($\alpha, \beta, \gamma \in \{x, y, z\}$, а $\epsilon_{\alpha\beta\gamma}$ – символ Леви-Чивиты).

• Они удобно экспоненциируются: $\exp(ian_\alpha\hat{\sigma}^\alpha) = \cos a + in_\alpha\hat{\sigma}^\alpha \sin a$ (тут $\vec{n}$ – произвольный единичный вектор). *Указание*: разложите экспоненту в ряд; из-за простого правила произведения матриц Паули, произвольные степени отих линейных комбинаций вычисляются достаточно просто.

Solution.

Матрицы Паули:

$$\hat{\sigma}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

• Проверим, что матрицы Паули являются линейно независимой системой от противного: предположим, что существуют a_0, a_1, a_2, $a_3 \in \mathbb{R}$:

$$a_0\hat{\sigma}^0 + a_1\hat{\sigma}^1 + a_2\hat{\sigma}^2 + a_3\hat{\sigma}^3 = 0$$

$$\begin{pmatrix} a_0 + a_3 & a_1 - ia_2 \\ a_1 + ia_2 & a_0 - a_3 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Единственное решение: $a_0 = a_1 = a_2 = a_3 = 0$, значит матрицы Паули действительно линейно независимы. Покажем, что любая эрмитова матрица 2×2 $B = (b_i)$ лежит в их линейной оболочке:

$$\begin{pmatrix} a_0 + a_3 & a_1 - ia_2 \\ a_1 + ia_2 & a_0 - a_3 \end{pmatrix} = \begin{pmatrix} b_1 & b_2 \\ b_3 & b_4 \end{pmatrix}$$

Заметим, что матрица слева (а значит и справа) является эрмитовой (на главной диагонали величины вещественные, на побочной – комплексно-сопряжённые). Единственное решение: $a_0 = \frac{b_1+b_4}{2}$, $a_1 = \frac{b_2+b_3}{2}$, $a_2 = \frac{i(b_2-b_3)}{2}$, $a_3 = \frac{b_1-b_4}{2}$. Таким образом, матрицы Паули совместно с единичной матрицей образуют базис в пространстве эрмитовых матриц 2×2.

• Проверим соотношения на матрицы Паули:

$$\sigma^1\sigma^1 = \sigma^2\sigma^2 = \sigma^3\sigma^3 = \mathbb{I}$$

$$\sigma^1\sigma^2 = -\sigma^2\sigma^1 = -i\sigma^3, \quad \sigma^1\sigma^3 = -\sigma^3\sigma^1 = -i\sigma^2, \quad \sigma^2\sigma^3 = -\sigma^3\sigma^2 = -i\sigma^1$$

Таким образом,

$$\hat{\sigma}^\alpha\hat{\sigma}^\beta = \delta_{\alpha\beta}\hat{\mathbb{I}} + i\epsilon_{\alpha\beta\gamma}\hat{\sigma}^\gamma$$

- $$\exp(ian_\alpha\hat{\sigma}^\alpha) = \sum_{k=0}^{\infty}\frac{(ian_\alpha\hat{\sigma}^\alpha)^k}{k!}$$

Найдём $(n_\alpha\hat\sigma^\alpha)^2$. Для этого воспользуемся правилом перемножения матриц Паули из п. 2:

$$n_\alpha\hat\sigma^\alpha n_\beta\hat\sigma^\beta = \hat{\mathbb{I}} + i\epsilon^{\alpha\beta\gamma}n_\alpha n_\beta\hat\sigma_\gamma = \hat{\mathbb{I}}$$

Из этого следует:

$$(n_\alpha\hat\sigma^\alpha)^{2k} = \hat{\mathbb{I}}, \quad (n_\alpha\hat\sigma^\alpha)^{2k+1} = n_\alpha\hat\sigma^\alpha, \quad k \in \{0\}\cup\mathbb{N}$$

$$\exp(ian_\alpha\hat\sigma^\alpha) = \sum_{k=0}^{\infty}\frac{(-1)^k a^{2k}(n_\alpha\hat\sigma^\alpha)^{2k}}{(2k)!} + i\sum_{k=0}^{\infty}\frac{(-1)^k a^{2k+1}(n_\alpha\hat\sigma^\alpha)^{2k+1}}{(2k+1)!}$$

$$\exp(ian_\alpha\hat\sigma^\alpha) = \mathbb{I}\sum_{k=0}^{\infty}\frac{(-1)^k a^{2k}}{(2k)!} + in_\alpha\hat\sigma^\alpha\sum_{k=0}^{\infty}\frac{(-1)^k a^{2k+1}}{(2k+1)!}$$

$$\exp(ian_\alpha\hat\sigma^\alpha) = \mathbb{I}\cos a + in_\alpha\hat\sigma^\alpha\sin a$$

ПТФ-3.з1. Каноническое квантование

Один из способов построения квантовой механики заключается в постулировании коммутационных соотношений, связанных с классической скобкой Пуассона: $[\hat A, \hat B] \to i\hbar\{\hat A, \hat B\}$; для канонически сопряжённых операторов координаты импульса это даёт $[\hat x, \hat p] = i\hbar$.

Пусть известно, что у оператора $\hat x$ имеется непрерывный спектр собственных значений $\mathbb{R}$, а также известны коммутационные соотношения $[\hat x, \hat p] = i\hbar$. Продемонстрируйте, что только этих знаний достаточно, чтобы вывести явный вид оператора импульса в координатном представлении $\hat p = -i\hbar\frac{\partial}{\partial x}$.

Дополнительно: покажите, что не существует конечномерных представлений этой алгебры: операторы $\hat x$ и $\hat p$, определённые таким образом, не могут действовать в гильбертовом пространстве конечной размерности.

Указания:

• Вычислите по индукции $[\hat x, \hat p^n]$.

• Оператор трансляции определим стандартным образом как $\hat T_a = e^{i\hat p a/\hbar}$. Используя предыдущий пункт, вычислите коммутатор $[\hat x, \hat T_a]$.

• Пусть $|x\rangle$ – базис собственных состояний оператора $\hat x$, так что $\hat x|x\rangle = x|x\rangle$. Покажите, что построенный оператор $\hat T_a$ действительно является оператором трансляции: $\hat T_a|x\rangle = |x-a\rangle$.

• Используя матричный элемент $\langle x|\hat T_a|\psi\rangle$ для инфинитезимальной трансляции $a \to 0$, найдите матричный элемент $\langle x|\hat p|\psi\rangle \equiv \hat p\psi(x)$.

Solution.

(допишу в пару строк основную идею)
Воспользуемся указаниями:
• Вычислим $[\hat x, \hat p^n]$ по индукции:

$$[\hat x, \hat p] = i\hbar$$

$$[\hat x, \hat p^n]\psi(x) \equiv \hat x\hat p^n\psi(x) - \hat p^n\hat x\psi(x) = \hat x\hat p^{n-1}\hat p\psi(x) - \hat p^{n-1}\hat p\hat x\psi(x) = \hat x\hat p^{n-1}\hat p\psi(x) - \\ - \hat p^{n-1}(\hat x\hat p - i\hbar)\psi(x) = [\hat x, \hat p^{n-1}]\hat p\psi(x) + i\hbar\hat p^{n-1}\psi(x)$$

$$[\hat x, \hat p^n] = i\hbar n\hat p^{n-1}$$

• Распишем оператор трансляции в ряд Тейлора:

$$\hat T_a = e^{i\hat p a/\hbar} = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\hat p a}{\hbar}\right)^n$$

$$[\hat x, \hat T_a] = \left[\hat x, \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\hat p a}{\hbar}\right)^n\right] = \sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{ia}{\hbar}\right)^n[\hat x, \hat p^n]$$

Воспользуемся предыдущим пунктом:

$$[\hat x, \hat T_a] = \sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{ia}{\hbar}\right)^n i\hbar n\hat p^{n-1} = -a\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{ia\hat p}{\hbar}\right)^n$$

$$[\hat x, \hat T_a] = -a\hat T_a$$

• Воспользуемся предыдущим пунктом:

$$[\hat{x}, \hat{T}_a]|x\rangle = -a\hat{T}_a|x\rangle$$

$$\hat{x}\hat{T}_a|x\rangle - \hat{T}_a\hat{x}|x\rangle = -a\hat{T}_a|x\rangle$$

$$\hat{x}\hat{T}_a|x\rangle = \hat{T}_a x|x\rangle - a\hat{T}_a|x\rangle = (x-a)\hat{T}_a|x\rangle$$

Как видно, действие оператора $\hat{x}$ на $|x-a\rangle$

$$\hat{x}|x-a\rangle = (x-a)|x-a\rangle$$

совпадает с действием на $\hat{T}_a|x\rangle$, следовательно

$$\hat{T}_a|x\rangle = |x-a\rangle$$

• Для инфинитезимальной трансляции $a \to 0$:

$$\langle x|\hat{T}_a|\psi\rangle = \langle x|\mathbb{I} + i\hat{p}a/\hbar|\psi\rangle = \psi(x) + \frac{ia}{\hbar}\hat{p}\psi(x)$$

$$\langle x|\hat{T}_a|\psi\rangle = \langle \hat{T}_a^\dagger x|\psi\rangle = \langle x+a|\psi\rangle = \psi(x+a) = \psi(x) + a\frac{\partial\psi(x)}{\partial x}$$

Сравнивая предущие равенства, получаем

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

Покажем, что не существует конечномерных представлений этой алгебры. От противного, предположим существуют представления $\hat{x}$ и $\hat{p}$ в виде матриц конечного размера $n \times n$.

$$\mathrm{tr}([\hat{x}, \hat{p}]_{n\times n}) = \mathrm{tr}(i\hbar\mathbb{I}_{n\times n}) = i\hbar n$$

$$\mathrm{tr}([\hat{x}, \hat{p}]_{n\times n}) = \mathrm{tr}(\hat{x}\hat{p} - \hat{p}\hat{x}) = 0$$

$i\hbar n \neq 0$, противоречие.

(??? вопрос в духе, что если взять поле чисел характеритики n, где $n \equiv 0$ - сложный вопрос и я даже не знаю, кто на него сможет ответить. Поэтому пока считаем, что такой вот ответ и все. см. мои последние главы, там когда-то обсужу этот вопрос)

ПТФ-3.з2. Преобразование Галлилея

Пусть частица находится в потенциале, который движется со скоростью v:

$$\hat{H}(t) = \frac{\hat{p}^2}{2m} + V(\hat{x} - vt)$$

Придумайте унитарное преобразование $\hat{U}(t)$ ("преобразование Галлилея"), которое приведёт Гамильтониан к аналогичному, но независящему от времени виду:

$$\hat{H}' \equiv \hat{U}(t)\hat{H}(t)\hat{U}^\dagger(t) - i\hbar\hat{U}(t)\partial_t\hat{U}^\dagger(t) = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

Запишите явно его действие на произвольную волновую функцию $\langle x|\hat{U}(t)|\psi(t)\rangle$.

Solution.

Избавимся от зависимости от времени в качестве преобразования при помощи оператора трансляции $\hat{T}_{vt}$:

$$\hat{T}_{vt} = \exp\left(vt\frac{\partial}{\partial x}\right) = \exp\left(\frac{ivt}{\hbar}\hat{p}\right), \quad \hat{T}_{vt}^\dagger = \hat{T}_{vt}^{-1} = \exp\left(-\frac{ivt}{\hbar}\hat{p}\right)$$

$$\hat{T}_{vt}(t)\hat{H}(t)\hat{T}_{vt}^\dagger(t) = \hat{T}_{vt}(t)\left(\frac{\hat{p}^2}{2m} + V(\hat{x} - vt)\right)\hat{T}_{vt}^\dagger(t) - i\hbar\hat{T}_{vt}(t)\partial_t\hat{T}_{vt}^\dagger(t)$$

Поскольку $\left[\hat{T}_{vt}(t), \frac{\hat{p}^2}{2m}\right] = 0$, то

$$\hat{T}_{vt}(t)\hat{H}(t)\hat{T}^{\dagger}_{vt}(t) = \frac{\hat{p}^2}{2m} + V(\hat{x}) - i\hbar \exp\left(\frac{ivt}{\hbar}\hat{p}\right)\left(-\frac{iv\hat{p}}{\hbar}\right)\exp\left(-\frac{ivt}{\hbar}\hat{p}\right) = \frac{\hat{p}^2}{2m} + V(\hat{x}) - v\hat{p}$$

Избавимся от слагаемого $-v\hat{p}$ при помощи оператора трансляции по импульсу:

$$\exp\left(a\frac{\partial}{\partial p}\right) = \exp\left(-\frac{ia\hat{x}}{\hbar}\right)$$

Поскольку $\left[\exp\left(-\frac{ia\hat{x}}{\hbar}\right), V(x)\right] = 0$, то

$$\exp\left(-\frac{ia\hat{x}}{\hbar}\right)\left(\frac{\hat{p}^2}{2m} + V(\hat{x}) - v\hat{p}\right)\exp\left(\frac{ia\hat{x}}{\hbar}\right) = \frac{(\hat{p}+a)^2}{2m} - v(\hat{p}+a) + V(\hat{x}) =$$
$$= \frac{\hat{p}^2}{2m} + \frac{a\hat{p}}{m} + \frac{a^2}{2m} - v\hat{p} - va + V(\hat{x})$$

Выберем $a = mv$:

$$\exp\left(-\frac{ia\hat{x}}{\hbar}\right)\left(\frac{\hat{p}^2}{2m} + V(\hat{x}) - v\hat{p}\right)\exp\left(\frac{ia\hat{x}}{\hbar}\right) = \frac{\hat{p}^2}{2m} - \frac{mv^2}{2} + V(\hat{x})$$

Избавимся от слагаемого $-\frac{mv^2}{2}$ при помощи оператора e^{ibt}, который коммутирует и с $\hat{x}$, и с $\hat{p}$:

$$\exp(ibt)\left(\frac{\hat{p}^2}{2m} - \frac{mv^2}{2} + V(\hat{x})\right)\exp(-ibt) - i\hbar\exp(ibt)(-ib)\exp(-ibt) = \frac{\hat{p}^2}{2m} - \frac{mv^2}{2} +$$
$$+ V(\hat{x}) - \hbar b$$

Выберем $b = -\frac{mv^2}{2\hbar}$. Таким образом, искомое унитарное преобразование:

$$U(t) = \exp\left(-\frac{imv^2t}{2\hbar}\right)\exp\left(-\frac{imv\hat{x}}{\hbar}\right)\exp\left(\frac{ivt\hat{p}}{\hbar}\right)$$

Подействуем оператором $\hat{U}(t)$ на функцию ψ:

$$\langle x|\hat{U}(t)|\psi(t)\rangle = \langle \hat{U}^{\dagger}(t)x|\psi(t)\rangle = \langle x+vt|\psi(t)\rangle \exp\left(-\frac{imv(x+vt)}{\hbar}\right)\exp\left(-\frac{imv^2t}{2\hbar}\right)$$

$$\langle x|\hat{U}(t)|\psi(t)\rangle = \psi(t, x+vt)\exp\left(-\frac{imv(x+vt)}{\hbar}\right)\exp\left(-\frac{imv^2t}{2\hbar}\right)$$

ФР. Оператор силы

Найти выражение для оператора силы

Solution..

(решение утеряно, напишу 1ю часть, потом пропишу это!)

Обсуждение (???)

(???? мы вообще можем использовать это выражение? проверю! укажу в теории его тоже!!!)

ФР. Момент силы

Найти выражение для оператора момента силы

Solution..

Воспользуемся $\hat{\dot{f}} = \frac{\partial \hat{f}}{\partial t} + \frac{i}{\hbar}\{\hat{H}, \hat{f}\}$, в нашем случае

$$\hat{\boldsymbol{M}}_\alpha = \epsilon_{\alpha\beta\gamma}\hat{\boldsymbol{r}}_\beta \hat{\boldsymbol{F}}_\gamma = \epsilon_{\alpha\beta\gamma}\hat{\boldsymbol{r}}_\beta \left(\frac{\partial \hat{p}}{\partial t} + \frac{i}{\hbar}\{\hat{H}, \hat{p}\}\right)$$

Ответ:

$$\hat{\boldsymbol{M}}_\alpha = \epsilon_{\beta\alpha\gamma}\hat{\boldsymbol{r}}_\beta \vec{\nabla}_\gamma U.$$

(решение не годящееся, потому что требуется из основ выводить. да? но ответ верный, да?)

ФР. Оператор дипольного момента

Найти выражение для оператора дипольного момента

Solution..

(решение утеряно, напишу 1ю часть, потом пропишу это!)

ФР. Найти выражение для оператора времени

Solution..

(??? ну тут проблема, конечно, в теории отдельный раздел про это напишу. пока оставил задачу.)

ФР. Найти выражение для оператора производной от дипольного момента

Solution..

(решение утеряно, напишу 1ю часть, потом пропишу это!)

Б-2.1.23 Расплывание волнового пакета

Используя оператор координаты свободной частицы в представлении Гейзенберга, найти закон движения и "расплывания" волнового пакета.

Solution..

(просто посмотрю ответы, слишком мало еще работал над этим, чтобы самому думать было легко.)

ПТФ-2.y1. (10 б). Среднее спина

Вычислите среднее значение спина $\langle \vec{S} \rangle$ и его дисперсию $\langle (\vec{S} - \langle \vec{S} \rangle)^2 \rangle$ для чистого $|\chi\rangle = \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}$ и смешанного $\hat{\rho} = \frac{\hat{\mathbb{P}}_\uparrow + \hat{\mathbb{P}}_\downarrow}{2}$ состояний спина $1/2$.

Комментарий: первая величина – это вектор, а вторая – это скаляр, длина вектора. *Указание*: Для частицы со спином $1/2$ (например, электрон) *оператор спина* (собственного момента) равен $\hat{\vec{S}} = \frac{\hbar}{2}\hat{\vec{\sigma}}$ (то есть $\hat{S}_x = (\hbar/2)\hat{\sigma}_x$ и т. д.).

Solution.

Решим упражнение для чистого состояния:

$$|\chi\rangle\langle\chi| = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$\langle \hat{S}_x \rangle = \mathrm{Tr}(|\chi\rangle\langle\chi|\hat{S}_x) = \frac{\hbar}{4}\mathrm{Tr}\left(\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right) = \frac{\hbar}{2}$$

$$\langle \hat{S}_y \rangle = \mathrm{Tr}(|\chi\rangle\langle\chi|\hat{S}_y) = \frac{\hbar}{4}\mathrm{Tr}\left(\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\right) = 0$$

$$\langle \hat{S}_z \rangle = \mathrm{Tr}(|\chi\rangle\langle\chi|\hat{S}_z) = \frac{\hbar}{4}\mathrm{Tr}\left(\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right) = 0$$

Среднее значение спина:

$$\langle \vec{S} \rangle = \frac{\hbar}{2}\begin{pmatrix}1\\0\\0\end{pmatrix}$$

$$\vec{S}^2 = \frac{\hbar^2}{4}(\sigma_x^2 + \sigma_y^2 + \sigma_z^2) = \frac{3\hbar^2}{4}$$

$$\langle \vec{S} \rangle^2 = \frac{3\hbar^2}{4}$$

Дисперсия:

$$\langle \vec{S}^2 \rangle - \langle \vec{S} \rangle^2 = \frac{\hbar^2}{2}$$

Решим упражнение для смешанного состояния:

$$\hat{\rho} = \frac{\hat{\mathbb{P}}_\uparrow + \hat{\mathbb{P}}_\downarrow}{2} = \frac{1}{2}(|\uparrow\rangle]\langle\uparrow| + |\downarrow\rangle]\langle\downarrow|) = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

$$\langle \hat{S}_x \rangle = \mathrm{Tr}(|\chi\rangle\langle\chi|\hat{S}_x) = \frac{\hbar}{4}\mathrm{Tr}\left(\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right) = 0$$

$$\langle \hat{S}_y \rangle = \mathrm{Tr}(|\chi\rangle\langle\chi|\hat{S}_y) = \frac{\hbar}{4}\mathrm{Tr}\left(\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\right) = 0$$

$$\langle \hat{S}_z \rangle = \mathrm{Tr}(|\chi\rangle\langle\chi|\hat{S}_z) = \frac{\hbar}{4}\mathrm{Tr}\left(\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right) = 0$$

Среднее значение спина:

$$\langle \vec{S} \rangle = 0$$

$$\vec{S}^2 = \frac{\hbar^2}{4}(\sigma_x^2 + \sigma_y^2 + \sigma_z^2) = \frac{3\hbar^2}{4}$$

$$\langle \vec{S} \rangle^2 = 0$$

Дисперсия:

$$\langle \vec{S}^2 \rangle - \langle \vec{S} \rangle^2 = \frac{3\hbar^2}{4}$$

19.1.2 Problems about formalism of second quantization

(похожее в конд средах. about how to construct, unsertand and extract basic physics from such models?)

19.1.3 Problems about Angular Momentum and Spin

ЛЛ3-54 Наклонная проекция спина

Частица со спином 1/2 находится в состоянии с определенным значением $s_z = 1/2$. Определить вероятности возможных значений проекции спина на ось z', наклоненную под углом θ к оси z.

Solution..

Средний вектор спина $\bar{\mathbf{s}}$ направлен, очевидно, по оси z и равен по величине 1/2. Проецируя его на ось z', найдем, что среднее значение спина в направлении z' есть $\bar{s}_{z'} = \frac{1}{2}\cos\theta$. С другой стороны, имеем $\bar{s}_{z'} = \frac{1}{2}w_+ - \frac{1}{2}w_-$, где $w_\pm$ - вероятности значений $s_{z'} = \pm 1/2$. Учитывая также, что $w_+ + w_- = 1$, получаем

$$w_+ = \cos^2(\theta/2), \quad w_- = \sin^2(\theta/2).$$

ЛЛ-28.1 Усреднение по l (?????)

Усреднить тензор $n_i n_k - \frac{1}{3}\delta_{ik}$ (где $\mathbf{n}$ - единичный вектор в направлении радиуса-вектора частицы) по состоянию с заданной абсолютной величиной вектора l, но не его направлением (т. е. неопределенным l_z).

Solution.

(???? видимо, я l не так глубоко еще понимаю??)

Искомое среднее значение есть оператор, который может выражаться лишь через оператор $\widehat{1}$. Ищем его в виде

$$\overline{n_i n_k} - \frac{1}{3}\delta_{ik} = a\left[\widehat{l}_i\widehat{l}_k + \widehat{l}_k\widehat{l}_i - \frac{2}{3}\delta_{ik}l(l+1)\right];$$

это есть наиболее общий вид составленного из компонент $\hat{\mathbf{l}}$ симметричного тензора второго ранга с равным нулю следом.

Для определения постоянной a умножаем написанное равенство слева на $\widehat{l}_i$, и справа на $\widehat{l}_k$ (с суммированием по i и k) (??? почему так??). Поскольку вектор $\mathbf{n}$ перпендикулярен к вектору $\hbar\widehat{\mathbf{l}} = [\widehat{\mathbf{r}}\widehat{\mathbf{p}}]$, то $n_i\widehat{l}_i = 0$. Произведение $\widehat{l}_i\widehat{l}_i\widehat{l}_k\widehat{l}_k = \left(\widehat{\mathbf{l}}^2\right)^2$ заменяем его собственным значением $l^2(l+1)^2$, а произведение $\widehat{l}_i\widehat{l}_k\widehat{l}_i\widehat{l}_k$ преобразуем с помощью соотношений коммутации (26.7) следующим образом:

$$\widehat{l}_i\widehat{l}_k\widehat{l}_i\widehat{l}_k = \widehat{l}_i\widehat{l}_i\widehat{l}_k\widehat{l}_k - ie_{ikl}\widehat{l}_i\widehat{l}_l\widehat{l}_k = \left(\widehat{\mathbf{l}}^2\right)^2 - \frac{i}{2}e_{ikl}\widehat{l}_i\left(\widehat{l}_l\widehat{l}_k - \widehat{l}_k\widehat{l}_l\right) =$$
$$= \left(\widehat{\mathbf{l}}^2\right)^2 + \frac{1}{2}e_{ikl}e_{lkm}\widehat{l}_i\widehat{l}_m = \left(\widehat{\mathbf{l}}^2\right)^2 - \widehat{\mathbf{l}}^2 = l^2(l+1)^2 - l(l+1)$$

(мы воспользовались $e_{ikl}e_{mkl} = 2\delta_{im}$). После простого приведения получим в результате

$$a = -\frac{1}{(2l-1)(2l+3)}$$

Б-2.4.1 Раскрытие коммутаторов

Раскрыть коммутаторы

а) $\left[\hat{l}_i, \hat{\mathbf{r}}^2\right]$; б) $\left[\hat{l}_i, \hat{\mathbf{p}}^2\right]$; в) $\left[\hat{l}_i, (\hat{\mathbf{r}}\mathbf{p})\right]$; г) $\left[\hat{l}_i, (\hat{\mathbf{p}}\hat{\mathbf{r}})\hat{\mathrm{p}}_k\right]$;

д) $\left[\hat{l}_i, \hat{\mathrm{p}}_k\hat{\mathrm{p}}_l\right]$; е) $\left[\hat{l}_z, \hat{l}_\pm\right]$; ж) $\left[\hat{I}_+, \hat{I}_-\right]$; з) $\left[\hat{l}_i, \hat{p}_k\right]$; и) $\left[\hat{l}_i, \hat{\mathrm{x}}_k\right]$; к) $\left[\hat{l}_i, f(r)\right]$.

Solution.

(потом подумаю еще раз)

2.4.1. а) 0 ; б) 0 ; в) 0 ; г) $i(\hat{\mathrm{p}}\hat{\mathrm{r}})e_{ikj}\hat{\mathrm{p}}_j$; д) $i\left(e_{ikj}\hat{\mathrm{p}}_j\hat{\mathrm{p}}_l + e_{ilj}\hat{\mathrm{p}}_k\hat{\mathrm{p}}_j\right)$; е) $\pm\hat{I}_{\pm}$;ж) $2\hat{I}_z$; 3) $ie_{ikj}\hat{\mathrm{p}}_j$; и) $ie_{ikj}\hat{x}_j$; к) 0.

Равенство нулю результатов в п.п. а), б), в), и к) связано с тем, что они отвечают коммутаторам $\hat{1}_i$ со скалярными операторами. Такие операторы не преобразуются при поворотах системы координат, а оператор $\hat{I}_i$ описывает преобразование векторов состояний именно при таких поворотах.

Одинаковая структура результатов в п.п. з) и и) есть следствие того, что $\hat{x}_k$ и $\hat{p}_k$ являются компонентами векторных операторов, т. е. преобразуются при поворотах, как компоненты векторов (см. также задачу 2.4.9).

Б-2.4.2 Следы (??)

Найти $\mathrm{Tr}\,\hat{l}_i$, используя коммутационные соотношения и свойство следа $\mathrm{Tr}(\hat{\mathrm{A}}\hat{\mathrm{B}}) = \mathrm{Tr}(\hat{\mathrm{B}}\hat{\mathrm{A}})$.

Solution.

(потом подумаю еще раз)

У нас оператор орбитального момента это как раз коммутатор, а след коммутатора равен нулю: $\mathrm{Tr}\,\hat{l}_i = 0$.

Б-2.4.3 Квадрат орбитального момента

Доказать, что собственные значения оператора $\hat{l}^2$ равны $l(l+1)$, исходя из того, что все координатные оси равноправны и возможные значения проекции m на данную ось равновероятны.

Solution.

Поскольку все оси координат равноправны, то

$$\langle \hat{\mathbf{I}}^2 \rangle = \langle \hat{I}_x^2 \rangle + \langle \hat{I}_y^2 \rangle + \langle \hat{I}_z^2 \rangle = 3\langle \hat{I}_z^2 \rangle.$$

Далее, исходя из равновероятности различных значений $\hat{l}_z$ имеем

$$\langle \hat{I}_z^2 \rangle = \frac{1}{2l+1} \sum_{m=-l}^{l} m^2 = \frac{2}{2l+1} \sum_{m=0}^{l} m^2 = \frac{l(l+1)}{3}.$$

Окончательно получаем, что $\mathbf{1}^2 = \langle \hat{I}^2 \rangle = l(l+1)$.

Б-2.4.4 Минимизация соотношением неопределённостей

Используя соотношение неопределённостей для $\hat{M}_x$ и $\hat{M}_y$, определить минимальное значение выражения

$$\langle l, l | \hat{M}_x^2 + \hat{M}_y^2 | l, l \rangle.$$

Solution.

Исходя из $\left[\hat{M}_x, \hat{M}_y\right] = i\hbar \hat{M}_z$ получаем (в соответствии с Б-2.1.9)

$$\langle \Delta \hat{M}_x^2 \rangle_{\min} \langle \Delta \hat{M}_y^2 \rangle_{\min} = \frac{\hbar^2}{4} \langle \hat{M}_z \rangle^2 = \frac{\hbar^2}{4} \hbar^2 l^2,$$

ибо усреднение проводится по состоянию $|l, l\rangle$. В силу симметрии задачи относительно осей x и y можно считать $\langle \Delta \hat{M}_x^2 \rangle_{\min} = \langle \Delta \hat{M}_y^2 \rangle_{\min}$, откуда

$$\langle \Delta \hat{M}_x^2 \rangle_{\min} = \frac{\hbar^2}{2} l,$$

Учитывая также, что $\langle \hat{M}_x \rangle = \langle \hat{M}_y \rangle = 0$ (см. Б-2.4.6), имеем $\langle \hat{M}_x \rangle$ и окончательно получаем

$$\langle l, l | \hat{M}_x^2 + \hat{M}_y^2 | l, l \rangle_{\min} = \hbar^2 \left(\frac{l}{2} + \frac{l}{2} \right) = \hbar^2 l$$

Б-2.4.5 Экспоненты и $\hat{l}$ (?)

Преобразовать оператор $e^{i\alpha L \hat{l}_z} \hat{l}_\pm e^{-i\alpha \hat{l}_z}$.

Solution.

(проделаю потом)
Использовать результаты задач 2.1.17 и 2.4.1.
Ответ: $e^{\pm i\alpha} \hat{I}_\pm$.

Б-2.4.6 Свойства проекций орбитального момента

Показать, что в состоянии $|l, m\rangle$ (определена проекция на ось z) выполняются соотношения:
а) $\langle \hat{I}_x \rangle = \langle \hat{I}_y \rangle = 0$;
б) $\langle \hat{I}_x \hat{I}_y \rangle = -\langle \hat{I}_y \hat{I}_x \rangle = \frac{im}{2}$
в) $\langle \hat{I}_x^2 \rangle = \langle \hat{I}_y^2 \rangle = \langle \Delta \hat{I}_x^2 \rangle = \frac{1}{2} \left[l(l+1) - m^2 \right]$.

Solution.

Поскольку

$$\hat{I}_{\pm}|l,m\rangle = \sqrt{l(l+1)-m(m\pm 1)}|l,m\pm 1\rangle$$

то $\langle \hat{I}_{\pm}\rangle \sim \langle l,m|l,m\pm 1\rangle = 0$. Отсюда получаем $\langle \hat{I}_x\rangle \pm i\langle \hat{I}_y\rangle = 0$, поэтому $\langle \hat{I}_x\rangle = \langle \hat{I}_y\rangle = 0$. Далее, из соотношения (1) имеем $\langle \hat{I}_{\pm}^2\rangle = 0$, откуда

$$\langle \hat{I}_x^2 - \hat{I}_y^2\rangle \pm i\langle \hat{I}_x\hat{I}_y + \hat{I}_y\hat{I}_x\rangle = 0,$$

и поэтому $\langle \hat{I}_x^2\rangle = \langle \hat{i}_y^2\rangle, \langle \hat{I}_x\hat{I}_y + \hat{I}_y\hat{I}_x\rangle = 0$. Исходя из этого и учитывая также, что $\langle \hat{I}_x\hat{I}_y - \hat{I}_y\hat{I}_x\rangle = i\langle \mathbb{1}_z\rangle$, получаем $\langle \hat{I}_x\hat{I}_y\rangle = -\langle \hat{I}_y\hat{I}_x\rangle = im/2$.

Из $\langle \hat{I}_x^2 + \hat{I}_y^2\rangle = \langle \hat{I}^2 - \hat{I}_z^2\rangle$, нетрудно получить утверждение в) данной задачи.

Б-2.4.7 Матрицы для $l = 1$

Для системы с $l = 1$ найти матрицы операторов $\hat{l}^2, \hat{l}_z, \hat{l}_+, \hat{l}_-, \hat{l}_x, \hat{l}_y$.

Solution.

Известно, что

$$\langle l,m'|\hat{1}_{\pm}|l,m\rangle = \sqrt{l(l+1)-m(m\pm 1)}\delta_{m',m\pm 1}.$$

Подставляя сюда разные для $l = 1$ разные m, получаем матрицы $\hat{l}_+, \hat{l}_-$, из них $\hat{l}_x, \hat{l}_y$. Также формулы $\langle l,m'|\hat{l}_z|l,m\rangle = m\delta_{m',m}$, и $\langle l,m'|\hat{\mathbb{1}}^2|l,m\rangle = l(l+1)\delta_{m',m}$ дают $\hat{l}^2$ и $\hat{l}_z$, которые диагональны. В итоге:

$$\hat{l}_+ = \sqrt{2}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{l}_- = \sqrt{2}\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\hat{l}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \hat{l}_y = \frac{i}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad \hat{l}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \hat{1}^2 = 2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Б-2.4.8

Найти собственные значения и собственные векторы оператора $\hat{\mathrm{j}}_n = (\hat{\mathrm{j}n})$ для квантовой системы с угловым моментом $j = 1$, где $\mathbf{n}$ - единичный вектор с составляющими $\mathbf{n} = \{\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta\}$.

Solution.

Б-2.4.9

Исходя из свойств оператора момента $\hat{\mathbf{j}}$ и векторного оператора $\hat{\mathbf{A}}$ при преобразованиях поворота, получить коммутационные соотношения

$$\left[\hat{\mathrm{j}}_i, \hat{\mathrm{A}}_k\right] = ie_{ikl}\hat{\mathrm{A}}_l.$$

Solution.

Б-2.4.10 Коммутаторы с $\hat{j}^2$

Доказать тождества

$$\left[\hat{\mathbf{j}}^2, \hat{\mathbf{A}}\right] = i\left(|\hat{\mathbf{A}}\times\hat{\mathbf{j}}] - [\hat{\mathbf{j}}\times\hat{\mathbf{A}}]\right);$$

$$\left[\hat{\mathbf{j}}^2, \left[\hat{\mathbf{j}}^2, \hat{\mathbf{A}}\right]\right] = 2\left(\hat{\mathbf{j}}^2\hat{\mathbf{A}} + \hat{\mathbf{A}}\hat{\mathbf{j}}^2\right) - 4\hat{\mathbf{j}}(\hat{\mathbf{j}}\hat{\mathbf{A}}),$$

где $\hat{\mathbf{j}}$ - оператор момента, а $\hat{\mathbf{A}}$ - произвольный векторный оператор, т. е. $\left[\hat{\mathrm{j}}_i, \hat{\mathrm{A}}_k\right] = ie_{ikl}\hat{\mathrm{A}}_l$.

Solution.

(как-то скучно это решать, когда-то порешаю, есть задачи интереснее и актуальнее)

Б-2.4.11 Найти собственные функции и собственные значения матриц Паули.

Solution.

(?? разве из определения это не очевидно?)

Б-2.4.12 Вектор поляризации

Вектор поляризации спина $\mathbf{P}$ определяется как вектор с компонентами $\mathrm{P}_i = \langle\hat{\sigma}_i\rangle = \langle\chi|\hat{\sigma}_i|\chi\rangle = \chi^+\hat{\sigma}_i\chi$, где χ - спиновая функция данного состояния. В состояниях а) $\chi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ и б) $\chi = \begin{pmatrix} \cos\theta/2 \\ e^{i\delta}\sin\theta/2 \end{pmatrix}$ найти P_i и $|\mathbf{P}|$.

Solution.

Б-2.4.13

Получить соотношение $\hat{\sigma}_i\hat{\sigma}_k = \hat{1}\delta_{ik} + ie_{ikl}\hat{\sigma}_l$.

Б-2.4.14

Доказать, что $(\hat{\sigma}\mathbf{A})(\hat{\sigma}\mathbf{B}) = (\mathbf{AB}) + i(\hat{\sigma}[\mathbf{A}\times\mathbf{B}])$, где $\mathbf{A}$ и $\mathbf{B}$ - обычные (не спиновые) векторные операторы.

Б-2.4.15

Вычислить $\hat{\sigma}_\pm^2$ и антикоммутаторы $\{\hat{\sigma}_\pm, \hat{\sigma}_x\}, \{\hat{\sigma}_\pm, \hat{\sigma}_y\}, \{\hat{\sigma}_\pm, \hat{\sigma}_z\}$.

Б-2.4.16

Вычислить $\mathrm{Tr}\,\hat{\sigma}_i\hat{\sigma}_k, \mathrm{Tr}\,\hat{\sigma}_i\hat{\sigma}_k\hat{\sigma}_l$.

Б-2.4.17

Вычислить $(\hat{\sigma}\mathbf{a})^k$, где $\mathbf{a}$ - обычный вектор.

Б-2.4.18

Найти явный вид оператора $\exp[i\alpha(\hat{\sigma}\mathbf{n})]$.

Б-2.4.19

Найти собственные значения и собственные функции спинового оператора $\hat{\sigma}_n = (\hat{\sigma}\mathbf{n}_0)$, где $\mathbf{n}_0$ - единичный вектор с составляющими $\mathbf{n}_0 = \{\sin\theta_0\cos\varphi_0, \sin\theta_0\sin\varphi_0, \cos\theta_0\}$.

Б-2.4.20 Поворот спинора

Записать оператор, преобразующий спинор (спиновую волновую функцию ψ) при повороте системы координат на угол α вокруг оси с направлением, заданным единичным вектором $\mathbf{n}$. Найти явный вид оператора преобразования спинора при повороте системы координат, при котором ось z совмещается с направлением $\mathbf{n}_0 = \{\sin\theta_0\cos\varphi_0, \sin\theta_0\sin\varphi_0, \cos\theta_0\}$.

Solution.

(!??!?!!! добавлю в 1ю часть это!!!)

Искомый оператор преобразования спинора имеет вид $\hat{R}(\alpha\mathbf{n}) = \exp\left[i\frac{\alpha}{2}(\hat{\sigma}\mathbf{n})\right]$ (см. (II.23)).

Для того, чтобы ось z оказалась совмещенной с направлением вектора $\mathbf{n}_0$, необходимо осуществить поворот системы координат на угол θ_0 вокруг оси с направлением, заданным единичным вектором n, лежащим в плоскости xOy, а также перпендикулярным оси z и вектору $\mathbf{n}_0$. Несложный расчет показывает, что $\mathbf{n} = \{-\sin\varphi_0, \cos\varphi_0, 0\}$. Поэтому матрица оператора преобразования спинора будет иметь вид

$$\hat{\mathrm{R}}\,(\theta_0\mathbf{n}) = \exp\left[i\frac{\theta_0}{2}(\hat{\sigma}\mathbf{n})\right] = \cos\frac{\theta_0}{2} - i\sin\frac{\theta_0}{2}\,(\sin\varphi_0\hat{\sigma}_x - \cos\varphi_0\hat{\sigma}_y) = \begin{pmatrix} \cos\frac{\theta_0}{2} & \sin\frac{\theta_0}{2}e^{-i\varphi_0} \\ -\sin\frac{\theta_0}{2}e^{i\varphi_0} & \cos\frac{\theta_0}{2} \end{pmatrix}.$$

Действуя оператором $\hat{\mathrm{R}}$ на функции $\Psi_{\pm1}$ предыдущей задачи, получим с точностью до общего фазового множителя $\chi_{\pm1/2}$ (см. (II.26)).

Б-2.4.21

Используя результат предыдущей задачи, найти волновые функции частицы со спином $1/2$ в случае, когда проекция ее спина на направление $\mathbf{n}_0 = \{\sin\theta_0\cos\varphi_0, \sin\theta_0\sin\varphi_0, \cos\theta_0\}$ равна соответственно $\pm1/2$. Сравнить с результатом задачи 2.4.19.

Solution.

Б-2.4.23 Два поворота

Используя результат задачи 2.4.20, решить следующую геометрическую задачу: система координат поворачивается на угол φ_1 вокруг оси $\mathbf{n}_1$ и затем на угол φ_2 вокруг оси $\mathbf{n}_2$. Найти угол и направление оси вращения для результирующего поворота.

Solution.

Б-2.4.24 Матрицы со спином 1

Записать спиновые матрицы $\hat{\mathrm{S}}_x, \hat{\mathrm{S}}_y, \hat{\mathrm{S}}_z$ для частицы со спином 1 (взяв в качестве базиса состояния с определенной проекцией спина на ось z).

Solution.

(это в 1й уже написано, но все-таки еще раз решу! как ничего не помня это найти? додумаю потом. мб так же, как и с орбитальным моментам, одинаковые ведь матрицы?)

Б-2.4.25 Проекции 3D спина (!??!?!??)

Используя матрицы $\hat{\mathrm{S}}_x, \hat{\mathrm{S}}_y, \hat{\mathrm{S}}_z$, найти для частицы со спином 1 спиновую функцию состояния, отвечающего проекции спина $+1$ на направление $\mathrm{n}_0 = \{\sin\theta_0\cos\varphi_0, \cdots\}$. Найти вероятности различных проекций на ось z в этом состоянии. Исследовать специально случай θ_0, близких к нулю и к π, а также к $\pi/2$. Чем отличаются при $\theta_0 = \pi/2$ состояния со спином вдоль оси $x\,(\varphi_0 = 0)$ и со спином по оси $y\,(\varphi_0 = \pi/2)$?

Solution.

(!! додумаю скоро!)

2.4.25. Спиновая функция состояния, отвечающая проекции спина $+1$ на ось $\mathbf{n_0}$, совпадает с функцией ψ_1, найденной в решении задачи 2.4.8 для орбитального момента $l = 1$. Вероятности различных проекций спина на ось z в этом состоянии:

$$w(\pm1) = \frac{1}{4}\,(1 \pm \cos\theta_0)^2\,, \quad w(0) = \frac{1}{2}\sin^2\theta_0.$$

При $\theta_0 \to 0$ и $\theta_0 \to \pi$ функция переходит в $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ и $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ - функции, описывающие состояния с проекцией спина на ось z, равной ± 1. При $\theta_0 \to \pi/2, \varphi_0 \to 0$ и $\varphi_0 \to \pi/2$ решение переходит в $\frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}$ и $\frac{1}{2}\begin{pmatrix} -i \\ \sqrt{2} \\ i \end{pmatrix}$ - функции, описывающие состояния, в которых проекция спина на оси x и у равна $+1$.

19.1.4 Problems about Mathematical Properties of Quantum Mechanical Operators

(начало белоусова и любого типичного курса)

Киселев-л2.1.2. Тождество с коммутаторами

Докажите операторное тождество $\mathrm{e}^{A} B \mathrm{e}^{-A} = B + \sum\limits_{n=1}^{\infty} \underbrace{[A,[A,...[A,B]...]]}_{n}$.

Solution..

Нам полезно рассмотреть операторную функцию $F(\lambda) := \mathrm{e}^{\lambda A} B \mathrm{e}^{-\lambda A}$, возьмем его производную по λ в нуле:

$$\left.\frac{\mathrm{d}^n F(\lambda)}{\mathrm{d}\lambda^n}\right|_{\lambda=0} = \left.\sum_{k=0}^{n} C_n^k A^k \mathrm{e}^{\lambda A} B \mathrm{e}^{-\lambda A} A^{n-k} (-1)^{n-k}\right|_{\lambda=0} = \sum_{k=0}^{n} C_n^k A^k B A^{n-k} (-1)^{n-k},$$

где $C_n^k = n!/k!(n-k)!$ - комбинаторное число вариантов дифференцирования, т. е. коэффициент бинома Ньютона.

Поэтому искомый оператор имеет вид:

$$\mathrm{e}^{A} B \mathrm{e}^{-A} = F(1) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{k=0}^{n} C_n^k A^k B A^{n-k} (-1)^{n-k}.$$

При $n = 0$ коэффициент C_0^0 равен 1 и

$$\sum_{k=0}^{0} A^k B A^{n-k} (-1)^{n-k} = B.$$

Докажем методом индукции равенство

$$\sum_{k=0}^{n} C_n^k A^k B A^{n-k} (-1)^{n-k} = \underbrace{[A,[A,...[A,B]...]}_{n}.$$

Действительно, при $n = 1$ находим тождество

$$\sum_{k=0}^{1} C_1^k A^k B A^{n-k} (-1)^{n-k} = -BA + AB \equiv [A,B].$$

Пусть при $n = m \geqslant 1$ верно равенство

$$\sum_{k=0}^{m} C_m^k A^k B A^{m-k} (-1)^{m-k} = \underbrace{[A,[A,...[A,B]...]}_{m},$$

тогда при $n = m+1$ заметим прежде всего, что $C_{m+1}^k = \frac{m!}{k!(m-k)!} \frac{(m+1-k)+k}{m+1-k} = C_m^k + C_m^{k-1}$, причем это тождество справедливо при $k = m+1$, когда следует положить $C_m^{m+1} = 0$, и при $k = 0$, когда мы полагаем

$C_m^{-1}=0$. (???? подумаю про это потом!!) Тогда

$$\sum_{k=0}^{m+1} C_{m+1}^k A^k B A^{m+1-k}(-1)^{m+1-k} = \sum_{k=0}^{m} C_m^k A^k B A^{m+1-k}(-1)^{m+1-k} + \sum_{k=1}^{m+1} C_m^{k-1} A^k B A^{m-(k-1)}(-1)^{m-(k-1)} =$$
$$= -\left(\sum_{k=0}^{m} C_m^k A^k B A^{m-k}(-1)^{m-k}\right) A + A\left(\sum_{k=0}^{m} C_m^k A^k B A^{m-k}(-1)^{m-k}\right) =$$
$$= [A, \underbrace{[A,[A,...[A,B]...]}_{m}] = \underbrace{[A,[A,...[A,B]...]}_{(m+1)},$$

т. е. мы получаем верное равенство. Таким образом, утверждение доказано.

Киселев-л2.1.3. Экспоненты и операторы

Докажите операторное тождество для любой операторной функции $F(B)$:

$$\mathrm{e}^{A} F(B) \mathrm{e}^{-A} = F\left(\mathrm{e}^{A} B \mathrm{e}^{-A}\right).$$

Solution..

Согласно общему определению функция от оператора записывается в виде ряда Тейлора

$$F(B) = \sum_{n=0}^{\infty} \frac{1}{n!} F^{(n)}(0) B^n,$$

так что рассмотрим выражение

$$\mathrm{e}^{A} B^n \mathrm{e}^{-A} = \underbrace{\mathrm{e}^{A} B \mathrm{e}^{-A} ... \mathrm{e}^{A} B \mathrm{e}^{-A}}_{n} = \left(\mathrm{e}^{A} B \mathrm{e}^{-A}\right)^n,$$

где мы учли, что $\mathrm{e}^{A}\mathrm{e}^{-A} = \mathbb{1}$. Значит, действительно,

$$\mathrm{e}^{A} F(B) \mathrm{e}^{-A} = \sum_{n=0}^{\infty} \frac{1}{n!} F^{(n)}(0) \left(\mathrm{e}^{A} B \mathrm{e}^{-A}\right)^n = F\left(\mathrm{e}^{A} B \mathrm{e}^{-A}\right)$$

(??? еще чуть подумаю об этом.)

Киселев-л2.1.4. Коммутаторы и перестановки

Докажите, что для операторов A и B, перестановочных со своим коммутатором $[A,B]$, имеют место равенства

$$\mathrm{e}^{A}\mathrm{e}^{B} = \mathrm{e}^{[A,B]}\mathrm{e}^{B}\mathrm{e}^{A}$$

и

$$\left(\mathrm{e}^{A}\mathrm{e}^{B}\right)^n = \mathrm{e}^{\frac{1}{2}n(n+1)[A,B]}\mathrm{e}^{nB}\mathrm{e}^{nA}.$$

Solution..

Известно, что для любой операторной функции $\mathrm{e}^{A} F(B) \mathrm{e}^{-A} = F\left(\mathrm{e}^{A} B \mathrm{e}^{-A}\right)$, поэтому

$$\mathrm{e}^{A}\mathrm{e}^{B} = \mathrm{e}^{A}\mathrm{e}^{B}\mathrm{e}^{-A}\mathrm{e}^{A} = \exp\left(\mathrm{e}^{A} B \mathrm{e}^{-A}\right)\mathrm{e}^{A}.$$

А также известно, что $\mathrm{e}^{A} B \mathrm{e}^{-A} = B + \sum_{n=1}^{\infty} \frac{1}{n!} \underbrace{[A,[A,...[A,B]...]}_{n}$, и тут по условию задачи обрывается на первом слагаемом:

$$\mathrm{e}^{A} B \mathrm{e}^{-A} = B + [A,B]$$

Поэтому,

$$\mathrm{e}^{A}\mathrm{e}^{B} = \mathrm{e}^{B+[A,B]}\mathrm{e}^{A} = \mathrm{e}^{[A,B]}\mathrm{e}^{B}\mathrm{e}^{A},$$

поскольку $[B,[A,B]] = [A,[A,B]] = 0$, и первая часть утверждения доказана.

(??? дальше я уже не соображаю, потом заново подумаю.)
Далее,

$$\left(\mathrm{e}^{A}\mathrm{e}^{B}\right)^{n}=\left(\mathrm{e}^{A}\mathrm{e}^{B}\right)^{n-1}\mathrm{e}^{A}\mathrm{e}^{B}=\left(\mathrm{e}^{A}\mathrm{e}^{B}\right)^{n-1}\mathrm{e}^{[A,B]}\mathrm{e}^{B}\mathrm{e}^{A}=\mathrm{e}^{[A,B]}\left(\mathrm{e}^{A}\mathrm{e}^{B}\right)^{n-1}\mathrm{e}^{B}\mathrm{e}^{A}.$$

Эту цепочку можно продолжить, поскольку аналогичным образом

$$\left(\mathrm{e}^{A}\mathrm{e}^{B}\right)^{n-1}\mathrm{e}^{B}\mathrm{e}^{A}=\mathrm{e}^{[A,B]}\left(\mathrm{e}^{A}\mathrm{e}^{B}\right)^{n-2}\mathrm{e}^{B}\left(\mathrm{e}^{A}\mathrm{e}^{B}\right)\mathrm{e}^{A}=\mathrm{e}^{2[A,B]}\left(\mathrm{e}^{A}\mathrm{e}^{B}\right)^{n-2}\mathrm{e}^{2B}\mathrm{e}^{2A}.$$

Уже доказано, что

$$\mathrm{e}^{A}\mathrm{e}^{kB}=\mathrm{e}^{k[A,B]}\mathrm{e}^{kB}\mathrm{e}^{A},$$

где k - число. Значит, продолжая понижать степень так, как это было сделано выше, находим

$$\left(\mathrm{e}^{A}\mathrm{e}^{B}\right)^{n}=\mathrm{e}^{\sum\limits_{k=1}^{m}k[A,B]}\left(\mathrm{e}^{A}\mathrm{e}^{B}\right)^{n-m}\mathrm{e}^{mB}\mathrm{e}^{mA}=\mathrm{e}^{\frac{1}{2}n(n+1)[A,B]}\mathrm{e}^{nB}\mathrm{e}^{nA},$$

где мы использовали известное выражение для суммы арифметической прогрессии.

Киселев-л2.1.5. Тождество Бейкера-Хаусдорфа

Докажите, что для операторов A и B, перестановочных со своим коммутатором $[A,B]$, имеет место тождество Бейкера-Хаусдорфа

$$\mathrm{e}^{A+B}=\mathrm{e}^{\frac{1}{2}[A,B]}\mathrm{e}^{B}\mathrm{e}^{A}.$$

Solution..

Вычислим $\exp(A+B)$ как предел

$$\mathrm{e}^{A+B}=\lim_{n\to\infty}\left(1+\frac{1}{n}(A+B)\right)^{n}=\lim_{n\to\infty}\left(\mathrm{e}^{A/n}\mathrm{e}^{B/n}\right)^{n},$$

где порядок сомножителей под знаком степени, конечно, можно было выбрать и обратным, что не умаляет общности дальнейшего рассмотрения. В предыдущей задаче мы показали, что

$$\left(\mathrm{e}^{A/n}\mathrm{e}^{B/n}\right)^{n}=\mathrm{e}^{\frac{1}{2}n(n+1)\frac{1}{n^2}[A,B]}\mathrm{e}^{B}\mathrm{e}^{A},$$

так что

$$\mathrm{e}^{A+B}=\lim_{n\to\infty}\mathrm{e}^{\frac{1}{2}n(n+1)\frac{1}{n^2}[A,B]}\mathrm{e}^{B}\mathrm{e}^{A}=\mathrm{e}^{\frac{1}{2}[A,B]}\mathrm{e}^{B}\mathrm{e}^{A}$$

Б-2.1.14

Раскрыть коммутаторы $\left[\hat{\mathrm{p}}_x,f(r)\right]$, $\left[\hat{\mathrm{p}}_x^2,f(r)\right]$, $\left[\hat{x},\exp\left(\frac{i}{\hbar}a\hat{\mathrm{p}}_x\right)\right]$, где $r=\sqrt{x^2+y^2+z^2}$.

Solution.

Б-2.1.15 оператор скорости

Получить выражение для оператора скорости частицы массы m.

Solution.

Б-2.1.16 Оператор эволюции и разная координата

Показать, что $\langle\mathbf{r}|U(\hat{\mathbf{r}})|\mathbf{r}'\rangle=U(\mathbf{r})\delta\left(\mathbf{r}-\mathbf{r}'\right)$.

Solution.

Б-2.1.17

Доказать справедливость соотношения ($[\hat{\mathrm{A}},\hat{\mathrm{B}}]\neq 0$)

$$e^{\xi\hat{\mathrm{A}}}\hat{\mathrm{B}}e^{-\xi\hat{\mathrm{A}}}=\hat{\mathrm{B}}+\xi[\hat{\mathrm{A}},\hat{\mathrm{B}}]+\frac{1}{2!}\xi^2[\hat{\mathrm{A}},[\hat{\mathrm{A}},\hat{\mathrm{B}}]]+...$$

Solution.

Б-2.1.18

Чему равен оператор

$$\exp\left(\frac{i}{\hbar}\mathbf{a}\hat{\mathbf{p}}\right)\hat{U}(\mathbf{r})\exp\left(-\frac{i}{\hbar}\mathbf{a}\hat{\mathbf{p}}\right),$$

где a - постоянный вектор?

Solution.

Б-2.1.19.

Оператор трансляции $\hat{T}_{\mathbf{a}}$ действует на векторы состояний с определенной координатой $|\mathbf{r}\rangle$ следующим образом: $\hat{T}_{\mathbf{a}}|\mathbf{r}\rangle = |\mathbf{r}-\mathbf{a}\rangle$. Как действует этот оператор на произвольный вектор состояния $|\psi\rangle$?

Solution.

19.1.5 Problems about Models of Many-Body Systems (!?!?!!)

Leuven-s7.ex3: Two fermions in a 1D well

Consider two spin- 1/2 particles in a one-dimensional infinite square well of size l ($V_{\text{pot}} = 0$ if $0 < x < L, \infty$ otherwise). The eigenfunctions and energies for the one particle problem are ($n > 0$)

$$u_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \quad E_n = n^2 E_1, \quad E_1 = \frac{\pi^2\hbar^2}{2mL^2}$$

(a) We neglect the interactions between the particles. Determine the three lowest energy levels.
(b) We suppose that the particles interact via the contact potential $V(x_1 - x_2) = g\delta(x_1 - x_2)$, where g does not depend on spin. Determine to first order in g the three lowest energy levels of this two-particles system.

Solutions:

(a) If we neglect the interaction, the energy is given by the sum of the 1 particle energies. The three lowest energy levels are

$$\begin{cases} 2E_1 & n_1 = 1, n_2 = 1 \\ 5E_1 & n_1 = 1, n_2 = 2 \text{ or } n_1 = 2, n_2 = 1 \\ 8E_1 & n_1 = 2, n_2 = 2 \end{cases}$$

The ground state being symmetric, the only allowed spin state is a singlet. Using the notation $|n, k; s, m_s\rangle$ for a general state (n and k can equivalently refer to n_1 or n_2), the ground state is given by $|1, 1; 0, 0\rangle$. The same is found for the second excited state. The first excited state, however, is neither symmetric or antisymmetric. We must thus construct the states coupled to a singlet and triplet states

$$|1, 2; 0, 0\rangle = \frac{1}{\sqrt{2}}\left(|n_1 = 1, n_2 = 2\rangle + |n_1 = 2, n_2 = 1\rangle\right)|s = 0, m_s = 0\rangle$$
$$|1, 2; 1, m_s\rangle = \frac{1}{\sqrt{2}}\left(|n_1 = 1, n_2 = 2\rangle + |n_1 = 2, n_2 = 1\rangle\right)|s = 1, m_s\rangle$$

(b) Since the perturbation does not depend on spin, we have for the ground state

$$\begin{aligned}\langle 1, 1; 0, 0|\hat{V}|1, 1; 0, 0\rangle &= \frac{4}{L^2}\iint \sin^2\left(\frac{\pi}{L}x_1\right)\sin^2\left(\frac{\pi}{L}x_2\right) g\delta(x_1 - x_2)\, dx_1 dx_2 \\ &= \frac{4}{L^2}g\int_0^L \sin^4\left(\frac{\pi}{L}x_1\right) dx_1\end{aligned}$$

We then find $\Delta_0^{(1)} = \frac{3g}{2L}$. We get exactly the same for the second excited state $\Delta_2^{(1)} = \frac{3g}{2L}$. For the first excited states, there is a degeneracy, because $|1, 2; 0, 0\rangle$ and $|1, 2; 1, m_s\rangle$ all have the same energy. However,

the perturbation does not affect the spin, so we can anticipate that it is already diagonal in the spin basis $\left(\langle 1,2;s,m_s|\hat{V}|1,2;s',m_s'\rangle = \langle 1,2|\hat{V}|1,2\rangle\langle s,m_s|s',m_s'\rangle \text{ with } \langle s,m_s|s',m_s'\rangle = \delta_{ss'}\delta_{m_s,m_s'}\right)$. The diagonal elements will then give the first-order energy shifts. For a triplet state, we have the diagonal elements

$$\begin{aligned}&\langle 1,2;1,m_s|\hat{V}|1,2;1,m_s\rangle \\ &= \frac{4}{L^2}\iint \frac{1}{2}\left[\sin\left(\frac{\pi}{L}x_1\right)\sin\left(\frac{2\pi}{L}x_2\right) - \sin\left(\frac{2\pi}{L}x_1\right)\sin\left(\frac{\pi}{L}x_2\right)\right]^2 g\delta\left(x_1-x_2\right)dx_1dx_2 = 0\end{aligned}$$

It makes sense since the triplet state does not allow for particles to be at the same position, so they will never feel the potential. For the singlet state, we have

$$|1,2;0,0|\hat{V}|1,2;0,0\rangle = \frac{4}{L^2}\frac{g}{2}\int_0^L 4\sin^2\left(\frac{\pi}{L}x_1\right)\sin^2\left(\frac{2\pi}{L}x_1\right)dx_1 = \frac{2g}{L}$$

So $\Delta_{1,\text{ triplet}} = 0$ and $\Delta_{1,\text{ singlet}} = 2g/L$.

19.2 Problems about Derivations of Properties

19.2.1 Problems about derivation of special constructions

Б-2.8.13 Вывод фазы Берри (??)

Квантовая система описывается гамильтонианом $\hat{\mathrm{H}}(\xi(t))$, зависящим от некоторого параметра $\xi(t)$, медленно (адиабатически) меняющегося во времени, так что в каждый момент времени имеем $\hat{H}(\xi(t))|\psi_n(\xi(t))\rangle = E_n(\xi(t))|\psi_n(\xi(t))\rangle$.

Показать, что для невырожденного уровня энергии $E_n(\xi(t))$ эволюция состояния во времени может быть представлена в виде

$$|\Psi_n(\xi(t))\rangle = e^{i\gamma(t)}e^{-\frac{i}{\hbar}\int_0^t E_n\left(\xi\left(t'\right)\right)dt'}|\psi_n(\xi(t))\rangle.$$

Получить уравнения для определения фазы γ и найти эту фазу (фаза Берри).

Solution.

Задача на воспроизведение известного теоретического результата.
(Maybe I'll just put it to the theory later, or focus more on technical side of it.)

Вначале рассмотрим динамическую часть фазы, приобретаемой вектором $|\psi_n(\xi(t))\rangle$ (см. условие задачи). Заметим, что временная эволюция состояния неконсервативной системы может быть представлена в виде

$$|\Psi(t)\rangle = \hat{\mathrm{U}}\left(t,t_0\right)|\Psi_0\rangle,$$

$$\hat{\mathrm{U}}\left(t,t_0\right) = \hat{\mathrm{T}}\exp\left(-\frac{i}{\hbar}\int_{t_0}^t \hat{\mathrm{H}}\left(\xi\left(t'\right)\right)dt'\right).$$

Пусть начальное состояние является одним из собственных векторов мгновенного гамильтониана в момент времени $t^{(n)}$, совпадающим с моментом времени оператора $\hat{\mathrm{H}}\left(t^{(n)}\right)$ в соответствующем n-м члене разложения правой части соотношения (1) (см. также (II.45)). Тогда оператор $\hat{\mathrm{H}}\left(t^{(n)}\right)$ может быть заменен соответствующим собственным значением энергии, а в силу невырожденности уровня энергии мгновенное состояние останется тем же самым. Поскольку параметр ξ изменяется во времени медленно, на интервале времени $\Delta t = t - t_0 \ll \tau$, где τ - характерное время изменения параметра, можно считать, что состояние будет близко к собственному состоянию для всех сомножителей членов ряда T exp. В этом случае действие оператора эволюции сводится к умножению исходного вектора состояния на фазовый множитель $\exp\left(-\frac{i}{\hbar}\int_0^t E_n\left(\xi\left(t'\right)\right)dt'\right)$. При этом в силу невырожденности уровня энергии состояние по-прежнему будет мгновенным собственным вектором гамильтониана в текущий момент времени.

Для интервала времени $\Delta t \geqslant \tau$ представим решение в виде, записанном в условии задачи, которое теперь должно удовлетворять уравнению Шредингера

$$i\hbar\frac{\partial}{\partial t}|\Psi(t,\xi(t))\rangle = \hat{\mathrm{H}}(\xi(t))|\psi(t,\xi(t))\rangle.$$

В силу того, что гамильтониан зависит от времени только через параметр $\xi(t)$,

$$i\hbar\frac{\partial}{\partial t}|\Psi(t,\xi(t))\rangle = \left[-\hbar j(t) + E_n(\xi(t))\right]|\Psi(t,\xi(t))\rangle + i\hbar\dot{\xi}(t)\left(\frac{\partial}{\partial\xi}|\psi_n(\xi(t))\rangle\right)e^{i\gamma(t)}e^{-\frac{i}{\hbar}\int E_0 E_n\left(\xi(t')\right)dt'}.$$

$$\frac{\partial}{\partial\xi}|\psi_n(\xi(t))\rangle = \sum_k |\psi_k(\xi(t))\rangle\langle\psi_k(\xi(t))|\frac{\partial}{\partial\xi}|\psi_n(\xi(t))\rangle \approx \langle\psi_n(\xi(t))|\frac{\partial}{\partial\xi}|\psi_n(\xi(t))\rangle|\psi_n(\xi(t))\rangle.$$

Здесь мы воспользовались адиабатическим приближением и опустили в сумме все слагаемые с $k \neq n$, имея в виду, что вероятности переходов в эти состояния экспоненциально малы. Таким образом, с учетом мгновенного стационарного уравнения Шредингера получаем

$$i\hbar\frac{\partial}{\partial t}|\Psi(t,\xi(t))\rangle = \left[-\hbar\dot{\gamma}(t) + i\hbar\dot{\xi}(t)\langle\psi_n(\xi(t))|\frac{\partial}{\partial\xi}|\psi_n(\xi(t))\rangle + E_n(\xi(t))\right]|\Psi(t,\xi(t))\rangle.$$

Поскольку уровень энергии $E_n(\xi(t))$ невырожден, состояние $|\Psi(t,\xi(t))\rangle$ также должно соответствовать этому же уровню энергии. Поэтому в правой части полученного уравнения можно заменить значение $E_n(\xi)$ действием гамильтониана $\hat{\mathrm{H}}(\xi)$. Таким образом, видим, что в правой части уравнения Шредингера появляются дополнительные члены, которые обязаны обратиться в нуль, что возможно при выполнении условия

$$\dot{\gamma}(t) = i\dot{\xi}(t)\langle\psi_n(\xi(t))|\frac{\partial}{\partial\xi}|\psi_n(\xi(t))\rangle.$$

Нетрудно показать, что функция $\dot{\gamma}(t)$ является действительной: продифференцируем условие нормировки $1 = \langle\psi_n(\xi)|\psi_n(\xi)\rangle$ и найдем соотношение

$$0 = \langle\psi_n(\xi)|\frac{\partial}{\partial\xi}|\psi_n(\xi)\rangle^* + \langle\psi_n(\xi)|\frac{\partial}{\partial\xi}|\psi_n(\xi)\rangle = 2\,\mathrm{Re}\left\{\langle\psi_n(\xi)|\frac{\partial}{\partial\xi}|\psi_n(\xi)\rangle\right\},$$

которое, по существу, и доказывает данное утверждение.

Если параметр ξ изменяется периодически с периодом T, описывая замкнутую траекторию в параметрическом пространстве, изменение фазы за период можно выразить через интеграл по замкнутому контуру Γ в параметрическом пространстве:

$$\gamma = \int_0^T dt\dot{\gamma}(t) = i\oint_\Gamma d\xi\langle\psi_n(\xi(t))|\frac{\partial}{\partial\xi}|\psi_n(\xi(t))\rangle.$$

19.3 Problems about Mathematical Quantum Mechanics

19.3.1 Problems about Mathematical Scattering

(add Takhtajayan in English here!!)

ЗАДАЧА 4.1. Докажите, что если

$$\sup_{\boldsymbol{x}\in\mathbb{R}^3}\int_{\mathbb{R}^3}|V(\boldsymbol{y})|\frac{1}{|\boldsymbol{x}-\boldsymbol{y}|}d^3\boldsymbol{y} < 4\pi$$

то интегральные уравнения Липпмана - Швингера можно решить с помощью ряда Неймана, а для фиксированных $\boldsymbol{x}$ и $\boldsymbol{\omega}$ решения $u^{(\pm)}(\boldsymbol{x},\boldsymbol{k})$, $\boldsymbol{k} = k\boldsymbol{\omega}$, допускают аналитическое продолжение в верхнюю полуплоскость $\mathrm{Im}\,k > 0$. Покажите также, что в этом случае у оператора Шрёдингера H нет собственных значений.

ЗАДАЧА 4.2 (БОРНОВСКОЕ ПРИБЛИЖЕНИЕ). Покажите, что $u^{(+)}(\boldsymbol{x},\boldsymbol{k}) = e^{i\boldsymbol{k}\boldsymbol{x}} + o(1)$ при $k\to\infty$, и выведите из этого, что

$$f(k,\boldsymbol{n},\boldsymbol{\omega}) + \frac{1}{4\pi}\int_{\mathbb{R}^3} e^{ik(\boldsymbol{n}-\boldsymbol{\omega})\boldsymbol{x}}V(\boldsymbol{x})d^3\boldsymbol{x} = o(1) \quad \text{при} \quad k\to\infty$$

равномерно на $\boldsymbol{n}, \omega \in S^2$.

ЗАдАЧА 4.3. Докажите унитарность оператора $\hat{S}$, используя уравнение Шрёдингера (4.6), условия излучения (4.7) и формулу Грина.

ЗАДАЧА 4.4 (ОПТИЧЕСКАЯ ТЕОРЕМА). ПокажИте, что

$$\int\limits_{S^2} |f(k, \boldsymbol{n}, \boldsymbol{\omega})|^2 d\boldsymbol{n} = \frac{4\pi}{k} \operatorname{Im} f(k, \boldsymbol{\omega}, \boldsymbol{\omega})$$

(Здесь левая часть - это полное сечение в направлении ω при энергии $E = k^2$)

ЗАДАЧА 4.5. Пусть $\lambda_l = -\varkappa_l^2 < 0$ - собственные значения H с кратностями $m_l, l = 1, ..., n$. Докажите, что для фиксированных $\boldsymbol{x}$ и $\boldsymbol{\omega}$ решения $u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k})$ допускают мероморфное продолжение в верхнюю полуплоскость $\operatorname{Im} k > 0$ с полюсами порядка m_l в точках $i\varkappa_l, l = 1, ..., n$.

ЗАДАЧА 4.6. Докажите, что волновые операторы $W_{\pm}$существуют, используя нестационарный подход. (Указание: покажите, что когда $V(\boldsymbol{x})$ удовлетворяет (4.5), применим критерий Кука, сформулированный в задаче 2.7.)

20 Other, Special Parts and Special Methods

20.1 Deep Understanding of Quantum Mechanics

20.1.1 Questions about the True Understanding of Quantum Mechanics

Приведем вопросы, которые покажут, понимает ли человек, что вообще происходит в квантмехе? Конечно же, это такие вопросы, ответы на которые приходят после лет размышлений, так что бессмысленно докапываться с ними до студентов, учащих квантовую механику первый год.

Я. Чем на самом деле квантовая физика отличается от классической

постановкой задачи, в квантовой - пучок траекторий,
в классической - одна
подробно про это.
(тут еще дисскуссия небольшая про неверные ответы)

Я. Откуда на самом деле появилось соотношение неопределённостей?

все его знают, однако четко указать, откуда - дело большое.
(тут еще дисскуссия небольшая про неверные ответы)

Я. Что необходимо для построения интеграла по траекториям?

тоже часто возникает вопрос.
(тут еще дисскуссия небольшая про неверные ответы)

Я. Почему некоторые квантовые системы не достигают равновесия?

(вообще не знаю, в интернете что-то про это было написано)
(тут еще дисскуссия небольшая про неверные ответы)

Я. Почему бы весь мир не описывался одним электроном в суперпозиции?

(?? мб можно что-то интересное сформулировать в рамках этой гипотезы? почитаю про это, если интересный вопрос, то оставлю тут, если нет - в конце записи вставлю.)

Я. Записывается ли информация о прошлом, или навсегда теряется? (???)

Если мы не можем отличить электроны, то казалось бы, информация теряется и прошлое полностью забывается? Или нет, в каких-то свойствах информацию о прошлом всегда можно найти?
(пока не знаю.)

Я. откуда появилась волновая функция

хз

Я. является ли оператор импульса самосопряженным?

Я. We measure some observable $\hat{A}$, what is the state of the system just after the measurement?

Казалось бы, в том же состоянии, где мы и измерили систему?
(??? надо бы это было еще продумать!)

Я. Why does non-degenerate perturbation theory break down if some states are degenerate?

(очень хороший типичный вопрос!)

20.1.2 Problems about Strict Mathematical Properties of Quantum Mechanics

(пока см. Тахтаджаян, добавлю их из других разделов)

20.1.3 Problems about Understanding the Details of the Mathematical Foundations of Quantum Mechanics

Приведем вопросы, которые покажут, понимает ли человек, как мы математически реализуем наше понимание квантовой механики?

Я. Матрицы канонических операторов, но с особой алгеброй

Могут ли существовать конечного размера матрицы, соответствующие координате и импульсу? Можно привести доказательство, что если взять след их коммутатора, то он равен нулю, а если взять след правой части, то получится всегда не ноль.

$$
\begin{aligned}
&[p;q] = i\hbar \\
&pq - qp = i\hbar \\
&t_2(pq - 4p) = i\hbar t_2 E \to \\
&t_2 py - t_7 qp = 0 = t_{11} E \cdot i\hbar \to 0
\end{aligned}
$$

Допустим можно взять поле чисел характиристики равной размерности пространства, тогда след единичной матрицы будет тоже ноль, и такое доказательство не работает. Спасает ли это эту ситуацию? Получается, что переходя к другому полю чисел можно сделать "квантовость" системы?

Solution

(Задачу очень на долго оставил, не актуально про это думать, да и не готов я к такому еще)

20.2 Special Theoretical Models

20.2.1 Problems about Open Systems

ПТФ-з1. Флуктуационно-диссипационная теорема (15 б).

Вне зависимости от происхождения индуцированного окружающей средой шума $\hat{\Phi}(t)$, на его корреляционные функции можно вывести соотношения самого общего вида, использующие лишь следующие общие предположения: гамильтониан $\hat{H}_e$ не зависит от времени; и матрица плотности окружающей среды имеет вид $\hat{\rho}_e = \frac{1}{Z} e^{-\beta \hat{H}_e}$.

• Используя формальное сходство между матрицей плотности и оператором эволюции в мнимом времени, покажите, что имеется связь на корреляционные функции $S_<(t) = S_>(t - i\beta)$. Что это означает для их фурье-образов, $S_<(\omega)$ и $S_>(\omega)$?

• Определим спектральную плотность как $J(\omega) = \frac{1}{2}(S_>(\omega) - S_<(\omega))$, и Келдышевский коррелятор как $S_K(t_1 - t_2) = \left\langle \left\{ \hat{\Phi}(t_1), \hat{\Phi}(t_2) \right\} \right\rangle$. Как связаны $S_K(\omega)$ и $J(\omega)$?

Solution

•

$$n_B(\omega) = \frac{1}{e^{\beta\omega} - 1}, \quad n_B(\omega) + 1 = -n_B(-\omega)$$

Корреляционные функции:

$$S_>(t) = \int\limits_0^\infty \frac{d\omega}{\pi} J(\omega)((n_B(\omega)+1)e^{-i\omega t} + n_B(\omega)e^{i\omega t}), \quad S_>(\omega) = 2\tilde{J}(\omega)(n_B(\omega)+1)$$

$$S_<(t) = \int\limits_0^\infty \frac{d\omega}{\pi} J(\omega)(n_B(\omega)e^{-i\omega t} + (n_B(\omega)+1)e^{i\omega t}), \quad S_<(\omega) = 2\tilde{J}(\omega)n_B(\omega)$$

где $\tilde{J}(\omega) = J(\omega) - J(-\omega)$.

$$S_>(t - i\beta) = \int\limits_0^\infty \frac{d\omega}{\pi} J(\omega)((n_B(\omega)+1)\exp(-i\omega t - \beta\omega) + n_B(\omega)\exp(i\omega t + \beta\omega)) =$$

$$= \int\limits_0^\infty \frac{d\omega}{\pi} J(\omega)\left(\frac{e^{\beta\omega}}{e^{\beta\omega}-1}e^{-i\omega t-\beta\omega} + \frac{1}{e^{\beta\omega}-1}e^{-i\omega t+\beta\omega}\right) = \int\limits_0^\infty \frac{d\omega}{\pi} J(\omega)\left(\frac{1}{e^{\beta\omega}-1}e^{-i\omega t} + \frac{e^{\beta\omega}}{e^{\beta\omega}-1}e^{-i\omega t}\right) =$$

$$= \int\limits_0^\infty \frac{d\omega}{\pi} J(\omega)(n_B(\omega)e^{-i\omega t} + (n_B(\omega)+1)e^{i\omega t}) = S_<(t)$$

$$S_>(t - i\beta) = S_<(t)$$

Покажем, что это означает для фурье-образов:

$$S_<(\omega) = \int\limits_{-\infty}^\infty dt S_<(t)e^{i\omega t} = \int\limits_{-\infty}^\infty dt S_>(t - i\beta)e^{i\omega(t-i\beta+i\beta)} = S_>(\omega)e^{-\omega\beta}$$

$$\frac{S_<(\omega)}{S_>(\omega)} = e^{-\omega\beta}$$

Это же равенство можно получить и из (**??**) и (**??**).

$$J(\omega) = \frac{1}{2}(S_>(\omega) - S_<(\omega))$$

$$S_K(t) = S_>(t) + S_<(t)$$

$$\frac{S_<(\omega)}{S_>(\omega)} = e^{-\omega\beta}$$

$$S_K(\omega) = 2J(\omega)\coth\left(\frac{\omega\beta}{2}\right)$$

ПТФ-з2. Релаксация (20 б).

Полученное на семинаре время релаксации T_1 для спин-бозонной модели, описываемой гамильтонианом

$$\hat{H} = -\frac{\Delta}{2}\hat{\sigma}_z + \sum_n \omega_n \hat{a}_n^\dagger \hat{a}_n + \hat{\sigma}_x\hat{\Phi}, \quad \hat{\Phi} = \sum_n \lambda_n(\hat{a}_n + \hat{a}_n^\dagger)$$

можно просто интерпретировать на языке золотого правила Ферми.

Solution

• Считая, что все осцилляторы находятся в квантовом состоянии с фиксированными числами заполнения n_n, вычислите частоту переходов $w_{i\to f} = w_{\uparrow\to\downarrow}$ и $w_{\downarrow\to\uparrow}$.

• Проведите усреднение полученных величин по Гиббсовскому ансамблю для осцилляторов $\hat{\rho}_e = \frac{1}{Z}e^{-\beta\hat{H}_e}$.

• Релаксационная динамика, описываемая золотым правилом Ферми, может быть сведена к классическому кинетическому уравнению:

$$\begin{cases} \frac{dP_\uparrow(t)}{dt} = -w_{\uparrow\to\downarrow}P_\uparrow(t) + w_{\downarrow\to\uparrow}P_\downarrow(t) \\ \frac{dP_\downarrow(t)}{dt} = -w_{\downarrow\to\uparrow}P_\downarrow(t) + w_{\uparrow\to\downarrow}P_\uparrow(t) \end{cases}$$

Исходя из такого уравнения, выразите время релаксации системы через величины $w_{\uparrow\to\downarrow}$ и $w_{\downarrow\to\uparrow}$ и сравните со временем релаксации, найденным на семинаре.

ПТФ-з3. Чистая дефазирока (50 б).

Исследуйте эволюцию матрицы плотности двухуровневой системы, взаимодействующую с резервуаром (набором осцилляторов). Система описывается следующим гамильтонианом:

$$\hat{H} = -\frac{\Delta}{2}\hat{\sigma}_z + \sum_n \omega_n \hat{a}_n^\dagger \hat{a}_n + \hat{\sigma}_z\hat{\Phi}, \quad \hat{\Phi} = \sum_n \lambda_n(\hat{a}_n + \hat{a}_n^\dagger)$$

• Перейдите к представлению взаимодействия. Оператор эволюции в представлении взаимодействия записывается при помощи $\mathcal{T}$-упорядоченной экспоненты:

$$\hat{S}(t,t_0) = \hat{\mathcal{T}}\left\{\exp\left(-i\int\limits_{t_0}^{t}\hat{V}(\tau)d\tau\right)\right\}$$

Гамильтониан в различные моменты времени не коммутирует сам с собой, поэтому $\mathcal{T}$-упорядочение убрать нельзя. Однако задачу можно значительно упростить, используя тот факт, что гамильтониан в различные моменты времени коммутирует на число:

$$[\hat{V}(t_1), \hat{V}(t_2)] = i\phi(t_1,t_2)$$

Используя этот факт, покажите, что знак $\mathcal{T}$-упорядочения можно снять ценой дополнительной добавки:

$$\hat{S}(t,t_0) = e^{i\Phi(t,t_0)}\exp\left(-i\int\limits_{t_0}^{t}\hat{V}(\tau)d\tau\right)$$

Указание: это соотношение можно вывести по индукции, рассмотрев $\hat{S}(t+\delta t,t_0) = \hat{S}(t+\delta t,t)\hat{S}(t,t_0)$ для $\delta t \to 0$, и объединив экспоненты при помощи формулы **Бейкера-Кэмбелла-Хаусдорфа**:

$$e^{\hat{A}}e^{\hat{B}} = \exp\left(\hat{A}+\hat{B}+\frac{1}{2}[\hat{A},\hat{B}]\right), \quad [\hat{A},\hat{B}] = \text{const}$$

• Пусть в начальный момент времени $t_0 = 0$ матрица плотности системы имела вид $\hat{\rho}_{tot}(t_0) = \hat{\rho}_s(t_0)\otimes\hat{\rho}_e(t_0)$, и резервуар находится в равновесии при температуре T: $\hat{\rho}_e(t_0) = \frac{1}{Z}e^{-\beta\hat{H}_0^{(e)}}$. Вычислите редуцированную матрицу плотности в произвольный момент времени:

$$\hat{\rho}_s(t) = \mathrm{Tr}_e(\hat{S}(t,t_0)\hat{\rho}_s(t_0)\hat{\rho}_e\hat{S}(t_0,t))$$

Указание: для усреднения по степеням бани вам может пригодиться тождество из задачи 6.1.

• Поскольку величина $\hat{\sigma}_z$ в данной задаче коммутирует с гамильтонианом, никакой релаксации наблюдаться не будет. Поэтому вся динамика сведётся к следующей временной зависимости матрицы плотности:

$$\hat{\rho}_s(t) = \begin{pmatrix} \rho_{11} & \rho_{12}\exp(-\Gamma(t)) \\ \rho_{21}\exp(-\Gamma(t)) & \rho_{22} \end{pmatrix}$$

Найдите выражение для **функции декогеренции** $\Gamma(t)$.

Solution

- Докажем соотношение $\hat{S}(t,t_0) = e^{i\Phi(t,t_0)} \exp\left(-i \int\limits_{t_0}^{t} \hat{V}(\tau) d\tau\right)$ по индукции.
- База индукции. Пусть соотношение верно для $t = t_0 + \delta t, \delta t \to 0$.

$$\hat{S}(t_0+\delta t, t_0) = e^{i\Phi(t_0+\delta t, t_0)} \exp\left(-i \int\limits_{t_0}^{t_0+\delta t} \hat{V}(\tau) d\tau\right) = \exp\left(-i \int\limits_{t_0}^{t_0+\delta t} \hat{V}(\tau) d\tau\right)$$

$$\Phi(t_0, t_0) = 0$$

- Пусть верно для момента t:

$$\hat{S}(t,t_0) = e^{i\Phi(t,t_0)} \exp\left(-i \int\limits_{t_0}^{t} \hat{V}(\tau) d\tau\right)$$

- Проверим, что выполняется для момента $t + \delta t$:

$$\hat{S}(t+\delta t, t_0) = e^{i\Phi(t,t_0)} \exp\left(-i \int\limits_{t_0}^{t+\delta t} \hat{V}(\tau) d\tau\right) =$$

$$= e^{i\Phi(t,t_0)} \exp\left(-i\hat{V}(t)\delta t\right) \exp\left(-i \int\limits_{t_0}^{t} \hat{V}(\tau) d\tau\right) =$$

$$= e^{i\Phi(t,t_0)} \exp\left(-i \int\limits_{t_0}^{t+\delta t} \hat{V}(\tau) d\tau - \frac{i}{2}\left[V(t)\delta t, \int\limits_{t_0}^{t} V(\tau) d\tau\right]\right) =$$

$$= e^{i\Phi(t,t_0) - \frac{i\delta t}{2}\int\limits_{t_0}^{t}\phi(t,\tau)d\tau} \exp\left(-i \int\limits_{t_0}^{t+\delta t} \hat{V}(\tau) d\tau\right) = e^{i\Phi(t+\delta t, t_0)} \exp\left(-i \int\limits_{t_0}^{t+\delta t} \hat{V}(\tau) d\tau\right)$$

$$\Phi(t+\delta t, t_0) = \Phi(t,t_0) - \frac{\delta t}{2} \int\limits_{t_0}^{t} \phi(t,\tau) d\tau \to \frac{d\Phi(t,t_0)}{dt} = -\frac{1}{2} \int\limits_{t_0}^{t} \phi(t,\tau) d\tau$$

$$\hat{S}(t,t_0) = e^{i\Phi(t,t_0)} \exp\left(-i \int\limits_{t_0}^{t} \hat{V}(\tau) d\tau\right), \quad \Phi(t,t_0) = -\frac{1}{2} \int\limits_{t_0}^{t} \int\limits_{t_0}^{\eta} \phi(\eta,\tau) d\tau d\eta$$

- Из определения коммутатора:

$$\phi(t_1,t_2) = -\phi(t_2,t_1) \to \Phi(t,0) = \Phi(-t,0)$$

$$\hat{\rho}_s(t) = \mathrm{Tr}_e(\hat{S}(t,t_0)\hat{\rho}_s(t_0)\hat{\rho}_e\hat{S}(t_0,t)) = e^{2i\Phi(t,t_0)}\mathrm{Tr}_e(e^{-i\int\limits_{t_0}^{t}\hat{V}(\tau)d\tau}\hat{\rho}_s(t_0)\hat{\rho}_e e^{i\int\limits_{t_0}^{t}\hat{V}(\tau)d\tau})$$

$$\hat{V} = \hat{\sigma}_z \sum_n \lambda_n (a_n e^{-i\omega_n t} + a_n^\dagger e^{i\omega_n t})$$

$$S = -i \int\limits_{t_0}^{t} \hat{V}(\tau) d\tau = \hat{\sigma}_z \sum_n \frac{\lambda_n}{\omega_n} (a_n(e^{-i\omega_n t_0} - e^{-i\omega_n t}) + a_n^\dagger (e^{i\omega_n t} - e^{i\omega_n t_0}))$$

$$\hat{\rho}_s(t) = e^{2i\Phi(t,t_0)}\mathrm{Tr}_e(e^S \hat{\rho}_s(t_0)\hat{\rho}_e e^{-S})$$

$$\hat{\rho}_s(t_0) = \begin{pmatrix}\rho_{11} & \rho_{12}\\ \rho_{21} & \rho_{22}\end{pmatrix} = \hat{\rho}_d + \rho_0, \quad \hat{\rho}_d = \begin{pmatrix}\rho_{11} & 0\\ 0 & \rho_{22}\end{pmatrix}, \quad \hat{\rho}_0 = \begin{pmatrix}0 & \rho_{12}\\ \rho_{21} & 0\end{pmatrix}$$

$$[\rho_d, \sigma_z] = 0 \to [\rho_d, e^S] = 0$$

$$e^{2i\Phi(t,t_0)}\mathrm{Tr}_e(e^S\hat\rho_d\hat\rho_e e^{-S}) = e^{2i\Phi(t,t_0)}\mathrm{Tr}_e(\hat\rho_d e^S\hat\rho_e e^{-S}) = \mathrm{Tr}_e(\hat\rho_d\hat S(t,t_0)\hat\rho_e\hat S(t_0,t)) =$$
$$= \mathrm{Tr}_e(\hat\rho_d\hat\rho_e(t)) = \hat\rho_d$$

$$\hat S = A\hat\sigma_z \to e^{\hat S} = \sum_n \frac{A^n}{n!}\hat\sigma_z^n = \sum_k \frac{A^{2k}}{(2k)!} + \sum_k \frac{A^{2k+1}}{(2k+1)!}\hat\sigma_z = \begin{pmatrix} e^A & 0 \\ 0 & e^{-A}\end{pmatrix}$$

$$e^{2i\Phi(t,t_0)}\mathrm{Tr}_e(e^S\hat\rho_0(t_0)e^{-S}e^S\hat\rho_e(t_0)e^{-S}) = \mathrm{Tr}_e(e^S\hat\rho_0(t_0)e^{-S}\hat\rho_e(t)) = \left\langle\begin{pmatrix} 0 & \rho_{12}e^{2A} \\ \rho_{21}e^{-2A} & 0\end{pmatrix}\right\rangle$$

$$\langle e^{2A}\rangle = e^{2\langle A^2\rangle}, \quad \langle a_n^\dagger a_n\rangle = n_B(\omega_n) = \frac{1}{e^{\beta\omega_n}-1}$$

$$\langle e^{2A}\rangle = \langle e^{-2A}\rangle = \exp\left(4\sum_n \frac{\lambda_n^2}{\omega_n^2}2\sin^2\frac{\omega_n(t-t_0)}{2}\coth\frac{\beta\omega_n}{2}\right)$$

$$\hat\rho_s(t) = \begin{pmatrix} \rho_{11} & \rho_{12}\exp\left(4\sum_n \frac{\lambda_n^2}{\omega_n^2}2\sin^2\frac{\omega(t-t_0)}{2}\coth\frac{\beta\omega_n}{2}\right) \\ \rho_{21}\exp\left(4\sum_n \frac{\lambda_n^2}{\omega_n^2}2\sin^2\frac{\omega(t-t_0)}{2}\coth\frac{\beta\omega_n}{2}\right) & \rho_{22}\end{pmatrix}$$

$$\hat\rho_s(t) = \begin{pmatrix} \rho_{11} & \rho_{12}\exp(-\Gamma(t)) \\ \rho_{21}\exp(-\Gamma(t)) & \rho_{22}\end{pmatrix}$$

Сравнивая с ответом из предыдущего пункта, получим

$$\Gamma(t) = -4\sum_n \frac{\lambda_n^2}{\omega_n^2}2\sin^2\frac{\omega_n(t-t_0)}{2}\coth\frac{\beta\omega_n}{2} = 4\sum_n \frac{\lambda_n^2}{\omega_n^2}(\cos\omega_n(t-t_0)-1)\coth\frac{\beta\omega_n}{2}$$

Спектральная плотность среды:

$$J(\omega) = \pi\sum_n \lambda_n^2\delta(\omega-\omega_n)$$

$t_0 = 0$.

$$\Gamma(t) = \frac{4}{\pi}\int_0^\infty d\omega J(\omega)\frac{\cos\omega t - 1}{\omega^2}\coth\frac{\omega}{2T}$$

ПТФ-з4 (15 б).

Используя функцию декогеренции из предыдущей задачи:

$$\Gamma(t) = \frac{4}{\pi}\int_0^\infty d\omega J(\omega)\coth\frac{\omega}{2T}\frac{1-\cos\omega t}{\omega^2},$$

исследуйте декогеренцию для омической бани, с модельной функцией $J(\omega) = \pi\alpha\omega e^{-\omega/\omega_c}$. Тут ω_c выступает в роли экспоненциальной ультрафиолетовой обрезки, и можно считать $\omega_c \gg T$. *Указание:* для вычисления удобно отделить вклад чисто квантовых флуктуаций (при $T = 0$), который зависит от обрезки ω_c; а затем найти температурный вклад, для которого обрезку уже можно выбросить.

Solution

Рассмотрим вклад чисто квантовых флуктуаций ($T = 0$):

$$\Gamma(t)\Big|_{T=0} = \frac{4}{\pi}\int_0^\infty d\omega\pi\alpha\omega e^{-\omega/\omega_c}\frac{1-\cos\omega t}{\omega^2} = 2\alpha\log(1+\omega_c^2t^2)$$

Температурный вклад ($T \neq 0$). Рассмотрим 2 случая:

- $Tt \gg 1$.

$$\Gamma(t) = 4\alpha\int_0^\infty d\omega\coth\left(\frac{\omega}{2T}\right)e^{-\frac{\omega}{\omega_c}}\frac{1-\cos\omega t}{\omega} \approx 4\alpha\int_0^\infty d\omega\frac{2T}{\omega}\frac{1-\cos\omega t}{\omega} = 4\pi\alpha tT$$

$$\Gamma(t) = 4\pi\alpha t T$$

- $Tt \ll 1$.

$$\frac{1-\cos\omega t}{\omega^2} \approx \frac{t^2}{2}$$

$$\Gamma(t) - \Gamma(t)\Big|_{T=0} = 4\alpha \int\limits_0^\infty d\omega \left(\coth\left(\frac{\omega}{2T}\right) - 1\right) e^{-\frac{\omega}{\omega_c}} \frac{1-\cos\omega t}{\omega} \approx$$

$$\approx 4\alpha \int\limits_0^\infty d\omega \left(\coth\left(\frac{\omega}{2T}\right) - 1\right) e^{-\frac{\omega}{\omega_c}} \frac{\omega t^2}{2} = 4\alpha t^2 \left(T^2\psi'\left(\frac{T}{\omega_c}\right) - \omega_c^2\right)$$

$$\Gamma(t) - \Gamma(t)\Big|_{T=0} \approx \frac{2\pi^2\alpha t^2 T^2}{3}$$

$$\Gamma(t) = 2\alpha\log(1+\omega_c^2 t^2) + \frac{2\pi^2\alpha t^2 T^2}{3}$$

ПТФ-15.з1. Модель Рубина (25 б).

Рассмотрите тяжёлую частицу массы M, которая соединена с баней, моделируемой одномерным полубесконечным кристаллом. В гармоническом приближении, система описывается следующим гамильтонианом:

$$\hat{H} = \frac{\hat{P}^2}{2M} + V(\hat{X}) + \sum_{n=1}^{\infty}\left(\frac{\hat{p}_n^2}{2m} + \frac{m\omega_0^2}{2}(\hat{u}_{n+1} - \hat{u}_n)^2\right) + \frac{m\omega_0^2}{2}(\hat{X} - \hat{u}_1)^2$$

Вычислите явный вид спектральной плотности $J(\omega)$, а также вид диссипативного ядра $\gamma(t)$.

Solution

$$\hat{H}_{\text{bath}} = \sum_{n=1}^{\infty}\left(\frac{\hat{p}_n^2}{2m} + \frac{m\omega_0^2}{2}(\hat{u}_{n+1} - \hat{u}_n)^2\right)$$

Пусть $\hat{u}_0 = 0$, $\hat{u}_{-i} = -\hat{u}_i$, тогда

$$\hat{u}_k = \sum_{l=-\infty}^{\infty} \hat{u}_n \sin kn, \quad \hat{p}_k = \sum_{l=-\infty}^{\infty} \hat{p}_n \sin kn$$

$$\hat{u}_n = \int\limits_0^\pi \frac{dk}{\pi}\hat{u}_k \sin kn, \quad \hat{p}_n = \int\limits_0^\pi \frac{dk}{\pi}\hat{p}_k \sin kn$$

$$\hat{H}_{\text{bath}} = \sum_{n=1}^{\infty}\int\limits_0^\pi\int\limits_0^\pi \frac{dkdk'}{\pi^2}\left(\frac{\hat{p}_k\hat{p}_{k'}\sin kn\sin k'n}{2m} + \frac{m\omega_0^2}{2}(\hat{u}_k\hat{u}_{k'}\sin kn\sin k'n + \right.$$

$$\left. + \hat{u}_k\hat{u}_{k'}\sin k(n+1)\sin k'(n+1) - 2\hat{u}_k\hat{u}_{k'}\sin k'n\sin k(n+1))\right)$$

$$\sin kn\sin k'n = \frac{1}{2}(\cos(k-k')n - \cos(k+k')n)$$

$$\sin k'n\sin k(n+1) = \frac{1}{2}(\cos((k'-k)n - k) - \cos((k'+k)n + k)) =$$

$$= \frac{1}{2}(\cos(k'-k)n\cos k - \sin(k'-k)n\cos k - \cos((k'+k)n+k))$$

$$\frac{1}{2\pi}\sum_{n=-\infty}^{\infty}\cos kn = \delta(k)$$

$$\hat{H}_{\text{bath}} = \int\limits_0^\pi \int\limits_0^\pi \frac{dkdk'}{\pi} \left(\frac{\hat{p}_k \hat{p}_{k'} \delta(k-k')}{2m} + \frac{m\omega_0^2}{2} 2\hat{u}_k \hat{u}_{k'} (1-\cos k) \right) =$$

$$= \int\limits_0^\pi \frac{dk}{\pi} \left(\frac{\hat{p}_k^2}{2m} + m\omega_0^2 \hat{u}_k^2 (1-\cos k) \right)$$

$$\hat{H}_{\text{int}} = \frac{m\omega_0^2}{2}(\hat{X}-\hat{u}_1)^2 - \frac{m\omega_0^2 \hat{u}_1^2}{2} = \frac{m\omega_0^2 \hat{X}}{2}(\hat{X}-2\hat{u}_1) = \int\limits_0^\pi \frac{dk}{\pi} \frac{m\omega_0^2 \hat{X}}{2}(\hat{X}-2\hat{u}_k \sin k)$$

$$\hat{H} = \frac{\hat{P}^2}{2M} + V(\hat{X}) + \int\limits_0^\pi \frac{dk}{\pi} \left(\frac{\hat{p}_k^2}{2m} + m\omega_0^2 \hat{u}_k^2 (1-\cos k) + \frac{m\omega_0^2 \hat{X}}{2}(\hat{X}-2\hat{u}_k \sin k) \right)$$

$$\hat{H} = \frac{\hat{P}^2}{2M} + V(\hat{X}) + \frac{m\omega_0^2 \hat{X}^2}{2} + \int\limits_0^\pi \frac{dk}{\pi} \left(\frac{\hat{p}_k^2}{2m} + m\omega_0^2 \hat{u}_k^2 (1-\cos k) - m\omega_0^2 \hat{X}\hat{u}_k \sin k) \right)$$

$$\hat{H} = \frac{\hat{P}^2}{2M} + V(\hat{X}) + \frac{m\omega_0^2 \hat{X}^2}{2} + \int\limits_0^\pi \frac{dk}{\pi} \left(\frac{\hat{p}_k^2}{2m} + \frac{m\omega^2(k)\hat{u}_k^2}{2} - c(k)\hat{X}\hat{u}_k) \right)$$

$$\omega(k) = 2\omega_0 \sin\frac{k}{2}, \quad c(k) = m\omega_0^2 \sin k$$

Спектральная плотность:

$$J(\omega) = \int\limits_0^\pi dk \frac{c^2(k)}{2m\omega(k)} \delta(\omega - \omega(k)) = \frac{m\omega_0^3}{4} \int\limits_0^\pi \frac{\sin^2 k}{\sin\frac{k}{2}} \delta\left(\omega - 2\omega_0 \sin\frac{k}{2}\right) dk =$$

$$= \frac{m\omega_0^3}{2} \int\limits_0^\pi dk \sin\frac{k}{2} \cos^2\frac{k}{2} \frac{\delta(k - 2\arcsin\frac{\omega}{2\omega_0})}{|\omega_0 \cos\frac{k}{2}|}$$

$$J(\omega) = \frac{m\omega_0\omega}{4} \sqrt{1 - \frac{\omega^2}{4\omega_0^2}} \theta\left(1 - \frac{\omega}{2\omega_0}\right)$$

Диссипативное ядро:

$$\gamma(t) = \frac{2}{\pi} \int\limits_0^\infty \frac{d\omega}{\omega} J(\omega) \cos\omega t = \frac{2}{\pi} \int\limits_0^{2\omega_0} d\omega \frac{m\omega_0}{4} \sqrt{1 - \frac{\omega^2}{4\omega_0^2}} \cos\omega t$$

$$\gamma(t) = \frac{m\omega_0}{4t} J_1(2\omega_0 t)$$

ПТФ-15.з2. Кинетическое уравнение (35 б).

Используя приближение Борна-Маркова для омической бани со спектральным весом $J(\omega) = \eta\omega$, выведите уравнение на преобразование Вигнера матрицы плотности $\rho_W(\mathbf{x}, \mathbf{p}, t)$.

ПТФ-15.з3. Расплывание волнового пакета (что, опять?) (40 б).

Упражнение. Преамбула (5 б).

Как известно из квантовой механики, волновые пакеты имеют обыкновение расплываться. С другой стороны, как известно, электрон имеет массу $m = 9.1 \cdot 10^{-28} g$, и его классический радиус $x_0 \simeq 10^{-13}$cm (определяемый как его комптоновская длина волны). Пусть в начальный момент времени электрон представлял собой ровно такой волновой пакет:

$$\psi(x) = \frac{1}{(2\pi x_0^2)^{1/4}} e^{-x^2/4x_0^2}$$

Найдите его ширину через время $t = 1\mu s$.

Solution

Перейдём в импульсное представление:

$$\Psi(p) = \int dx e^{-\frac{ipx}{\hbar}} \psi(x) = (8\pi x_0^2)^{\frac{1}{4}} e^{-\frac{p^2 x_0^2}{\hbar^2}}$$

Нестационарное уравнение Шрёдингера в импульсном представлении:

$$i\hbar \frac{\partial \Psi(p,t)}{\partial t} = \langle p|\hat{H}(t)|\psi(t)\rangle = \frac{p^2}{2m}\Psi(p,t), \quad \Psi(p,0) = \Psi(p)$$

$$\Psi(p,t) = \Psi(p) \exp\left(-\frac{ip^2}{2m\hbar}t\right)$$

$$\psi(x,t) = \int dx e^{\frac{ipx}{\hbar}} \Psi(p,t) = \left(\frac{2}{\pi}\right)^{\frac{1}{4}} \frac{\exp\left(-\frac{x^2}{4(x_0^2 + \frac{i\hbar}{2m}t)}\right)}{\sqrt{2x_0 + \frac{i\hbar t}{m x_0}}}$$

$$\mathrm{Re}\left(\frac{1}{x_0^2 + \frac{i\hbar t}{2m}}\right) = \mathrm{Re}\left(\frac{x_0^2 - \frac{i\hbar t}{2m}}{x_0^4 + \frac{\hbar^2 t^2}{4m^2}}\right) = \frac{1}{x_0^2 + \frac{\hbar^2 t^2}{4m^2 x_0^2}}$$

$$\Delta x^2(t) = x_0^2 + \frac{\hbar^2 t^2}{4m^2 x_0^2} \approx \frac{\hbar^2 t^2}{4m^2 x_0^2}$$

$$\Delta x(t) = \frac{\hbar t}{2m x_0} = 5.8 \cdot 10^6 \mathrm{cm}$$

ПТФ-15.з(35 б).

В предыдущем упражнении вы должны были получить ответ, который должен был вас удивить и насторожить. Рассмотрите теперь движение свободного электрона, взаимодействующего с окружающей средой в рамках модели Калдейры-Леггетта с омической баней. Получите асимптотические выражения для $\langle \hat{x}^2(t)\rangle$ в следующих режимах:
• Классическая диффузия: $Tt \gg 1$
• Квантовая диффузия: $Tt \ll 1$
Чтобы не рассматривать баллистические эффекты, оценённые в преамбуле, можете также считать $\omega_c \gg \gamma \gg t^{-1}$.

Solution

$$m\ddot{x} + \eta\dot{x} = \zeta(t) \to m\dot{v} + \eta v = \zeta(t)$$

$$v(t) = e^{-\frac{\eta t}{m}} \left(v_0 + \int_0^t d\tau \frac{\zeta(\tau)}{m} e^{\frac{\eta\tau}{m}}\right), \quad v(0) = 0$$

$$\dot{x}^2(t) = e^{-\frac{2\eta t}{m}} \int_0^t d\tau_1 \int_0^t d\tau_2 \frac{e^{\frac{\eta(\tau_1+\tau_2)}{m}}}{m^2} \zeta(\tau_1)\zeta(\tau_2)$$

20.2.2 Problems about the Functional Integral

ПТФ-16.у(10 б).

Восстановите координатную зависимость пропагатора квантового гармонического осциллятора $G(x,y,T)$. Исходя из полученного выражения, найдите его спектр.

Solution

Лагранжиан гармонического осциллятора:

$$L = \frac{m}{2}(\dot{x}^2 - \omega^2 x^2)$$

$$G^R(x,y,T) = \int\limits_{x(0)=x}^{x(T)=y} \mathcal{D}[x(t)] e^{\frac{iS[x(t)]}{\hbar}}, \quad \mathcal{D}[x(t)] = \left(\frac{m}{2\pi i\epsilon}\right)^{\frac{N}{2}} \prod_{k=1}^{N-1} \int dx_k$$

Сделаем подстановку в функциональный интеграл $x(t) = x_{\text{cl}}(t) + z(t)$, где $x_{\text{cl}}(t)$ – классическая траектория, удовлетворяющая граничным условиям $x_{\text{cl}}(0) = x$, $x_{\text{cl}}(T) = y$, $z(t)$ – произвольная функция (квантовая поправка) с граничными условиями $z(0) = 0$, $z(T) = 0$. Для систем, у которых действие зависит от x квадратично, выполняется

$$S[x(t)] = S[x_{\text{cl}}(t)] + S[z(t)]$$

$$S[x(t)] = \int\limits_0^T dt \frac{m}{2}(\dot{x}(t)^2 - \omega^2 x(t)^2) = \frac{m}{2}\left(x(t)\dot{x}(t)|_0^T - \int\limits_0^T dt x(t)(\ddot{x}(t) + \omega^2 x(t))\right)$$

Пусть $\hat{L} = -\partial_t^2 - \omega^2$, тогда

$$S[x(t)] = \frac{m}{2}\left(x(t)\dot{x}(t)|_0^T + \int\limits_0^T dt x\hat{L}x\right)$$

Поскольку на классической траектории $\hat{L}x_{\text{cl}}(t) = 0$, то в случае $x = y = 0$ выполняется $S[x_{\text{cl}}(t)] = 0$ и

$$G^R(0,0,T) = \int\limits_{x(0)=0}^{x(T)=0} \mathcal{D}[z(t)] e^{\frac{iS[z(t)]}{\hbar}} \to G^R(x,y,T) = G^R(0,0,T) e^{\frac{iS[x_{\text{cl}}(t)]}{\hbar}}$$

Определим действие на классической траектории:

$$\hat{L}x_{\text{cl}}(t) = 0 \to x_{\text{cl}}(t) = a\sin\omega t + b\cos\omega t$$

$$x_{\text{cl}}(0) = b = x, \quad x_{\text{cl}}(T) = a\sin\omega T + b\cos\omega T = y$$

$$x_{\text{cl}}(t) = \frac{y - x\cos\omega T}{\sin\omega T}\sin\omega t + x\cos\omega t, \quad \dot{x}_{\text{cl}}(t) = \frac{y - x\cos\omega T}{\sin\omega T}\omega\cos\omega t - x\omega\sin\omega t$$

$$S[x_{\text{cl}}(t)] = \frac{m}{2}(x_{\text{cl}}(T)\dot{x}_{\text{cl}}(T) - x_{\text{cl}}(0)\dot{x}_{\text{cl}}(0)) = \frac{m}{2}\left(\frac{y - x\cos\omega T}{\sin\omega T} y\omega\cos\omega T - xy\omega\sin\omega T - \right.$$
$$\left. - \frac{y - x\cos\omega T}{\sin\omega T} x\omega\right) = \frac{m\omega}{2}\frac{y^2\cos\omega T - xy\cos^2\omega T - xy\sin^2\omega T - yx + x^2\cos\omega T}{\sin\omega T} =$$
$$= \frac{m\omega}{2}\frac{(x^2+y^2)\cos\omega T - 2xy}{\sin\omega T}$$

Разложим произвольную функцию $z(t)$ по базису собственных функций оператора $\hat{L}$:

$$z(t) = \sum_n c_n z_n(t), \quad \hat{L}z_n(t) = \lambda_n z_n(t)$$

$$z_n(t) = \sqrt{\frac{2}{T}}\sin\frac{\pi n t}{T}, \quad \lambda_n = \frac{\pi^2 n^2}{T^2} - \omega^2$$

$$\mathcal{D}[z(t)] = \mathcal{N}\prod_{n=1}^{\infty}\int\limits_{-\infty}^{\infty} dc_n$$

$$S[z(t)] = S\left[\sum_n c_n z_n(t)\right] = \frac{m}{2}\int\limits_0^T dt\left(\sum_n c_n z_n(t)\right)\hat{L}\left(\sum_n c_n z_n(t)\right)$$

В силу ортонормированности набора $z_n(t)$ действие факторизуется:

$$S[z(t)] = \frac{m}{2}\int\limits_0^T dt\left(\sum_n c_n^2\lambda_n z_n^2(t)\right) = \frac{m}{2}\sum_{n=1}^{\infty}\lambda_n c_n^2$$

$$G_\omega^R(0,0,T) = \mathcal{N}\int\limits_{-\infty}^{\infty}\prod_{n=1}^{\infty}dc_n\exp\left(\frac{im}{2\hbar}\lambda_n c_n^2\right) = \mathcal{N}\prod_{n=1}^{\infty}\sqrt{\frac{2\pi i\hbar}{m\left(\frac{\pi^2n^2}{T^2}-\omega^2\right)}}$$

$$G_0^R(0,0,T) = \mathcal{N}\prod_{n=1}^{\infty}\sqrt{\frac{2\pi i\hbar T^2}{m\pi^2n^2}}$$

$$\frac{G_\omega^R(0,0,T)}{G_0^R(0,0,T)} = \prod_{n=1}^{\infty}\left(1-\frac{\omega^2T^2}{\pi^2n^2}\right)^{-\frac{1}{2}} = \sqrt{\frac{\omega T}{\sin\omega T}},\quad G_0^R(0,0,T) = \sqrt{\frac{m}{2\pi i\hbar T}}$$

$$G_\omega^R(0,0,T) = \sqrt{\frac{m}{2\pi i\hbar T}}\sqrt{\frac{\omega T}{\sin\omega T}} = \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}$$

$$G_\omega^R(x,y,T) = \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}\exp\left(\frac{im\omega((x^2+y^2)\cos\omega T-2xy)}{2\hbar\sin\omega T}\right)$$

Из знания запаздывающего пропагатора можно извлечь спектр гамильтониана.

$$G_\omega^R(x,y,T) = \langle y|e^{-\frac{i\hat{H}T}{\hbar}}|x\rangle = \sum_n\langle y|n\rangle e^{-\frac{iE_nT}{\hbar}}\langle n|x\rangle = \sum_n\psi_n^*(x)\psi_n(y)e^{-\frac{iE_nT}{\hbar}}$$

Воспользуемся разложениями:

$$\frac{1}{\sqrt{2i\sin\omega T}} = e^{-\frac{i\omega T}{2}}\sum_{n=0}^{\infty}C_{-\frac{1}{2}}^n e^{-2ni\omega T},\quad -\frac{i}{2\sin\omega T} = e^{-i\omega T}\sum_{n=0}^{\infty}e^{-2ni\omega T}$$

$$i\cot\omega T = -\frac{1+e^{-2i\omega T}}{1-e^{-2i\omega T}} = -\left(1+e^{-2i\omega T}\right)\sum_{n=0}^{\infty}e^{-2ni\omega T} = -2\sum_{n=0}^{\infty}e^{-2in\omega T}$$

$$G_\omega^R(x,y,T) = \sqrt{\frac{m\omega}{2\pi\hbar}}e^{-\frac{i\omega T}{2}}\left(\sum_{n=0}^{\infty}C_{-\frac{1}{2}}^n e^{-2i\omega nT}\right)\sum_{q=0}^{\infty}\frac{1}{q!}\left(\frac{m\omega}{\hbar}\right)^q\left(-(x^2+y^2)\left(\sum_{j=0}^{\infty}e^{-2i\omega jT}\right)+\right.$$
$$\left.+2xye^{-i\omega T}\sum_{j=0}^{\infty}e^{-2i\omega jT}\right)^q$$

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right)$$

Также получим спектр, рассмотрев следующую величину

$$\mathrm{Tr}\,G_\omega^R(x,y,T) = \int\limits_{-\infty}^{\infty}dxG_\omega^R(x,x,T) = \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}\int\limits_{-\infty}^{\infty}\exp\left(\frac{im\omega x^2}{\hbar\sin\omega T}\left(\cos\omega T-1\right)\right)dx =$$
$$= \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}\sqrt{\frac{\hbar\sin\omega T}{m\omega(1-\cos\omega T)}}\sqrt{\pi}e^{-i\pi/4} = \frac{1}{2i}\frac{1}{\sin\frac{\omega T}{2}} = e^{-\frac{i\omega T}{2}}\sum_{n=0}^{\infty}e^{-i\omega nT} = \sum_{n=0}^{\infty}e^{-\frac{iE_nT}{\hbar}}$$

ПТФ-16.з1. Пропагатор свободной частицы (15 б).

Вычислите интеграл для запаздывающего пропагатора свободной частицы явно, используя дискретизацию по времени:

$$G(x,y,t>0) = \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{N}{2}}\int\prod_{k=1}^{N-1}dx_k\exp\left(i\epsilon\sum_{k=1}^{N}\frac{m}{2\hbar}\left(\frac{x_k-x_{k-1}}{\epsilon}\right)^2\right),\quad x_0\equiv x,\quad x_N\equiv y$$

Solution

Вычислим интеграл по индукции.

$$\sqrt{\frac{m}{2\pi\hbar i\epsilon}}\int\limits_{-\infty}^{\infty}\exp\left(\frac{mi}{2\hbar\epsilon}((x_2-x_1)^2+(x_1-x_0)^2)\right)dx_1=$$

$$=\sqrt{\frac{m}{2\pi\hbar i\epsilon}}\int\limits_{-\infty}^{\infty}\exp\left(\frac{mi}{2\pi\hbar\epsilon}\left(2\left(x_1-\frac{x_0+x_2}{2}\right)^2+\frac{(x_2-x_0)^2}{2}\right)\right)dx_1=\frac{\exp(\frac{mi}{2\cdot2\hbar\epsilon}(x_2-x_0)^2)}{\sqrt{2}}$$

$$\sqrt{\frac{m}{2\cdot2\pi\hbar i\epsilon}}\int\limits_{-\infty}^{\infty}\exp\left(\frac{mi}{2\hbar\epsilon}\left((x_3-x_2)^2+\frac{(x_2-x_0)^2}{2}\right)\right)dx_2=$$

$$=\sqrt{\frac{m}{2\cdot2\pi\hbar i\epsilon}}\int\limits_{-\infty}^{\infty}\exp\left(\frac{mi}{2\hbar\epsilon}\left(\frac{3}{2}\left(x_2-\frac{x_0+2x_3}{9}\right)^2+\frac{(x_3-x_0)^2}{3}\right)\right)dx_2=$$

$$=\frac{\exp(\frac{mi}{2\cdot3\hbar\epsilon}(x_3-x_0)^2)}{\sqrt{3}}$$

Для k-го интеграла получим

$$\sqrt{\frac{m}{2k\pi\hbar i\epsilon}}\int\limits_{-\infty}^{\infty}\exp\left(\frac{mi}{2\hbar\epsilon}\left((x_{k+1}-x_k)^2+\frac{(x_k-x_0)^2}{k}\right)\right)dx_k=$$

$$=\sqrt{\frac{m}{2k\pi\hbar i\epsilon}}\int\limits_{-\infty}^{\infty}\exp\left(\frac{mi}{2\hbar\epsilon}\left(\frac{k+1}{k}\left(x_k-\frac{kx_{k+1}+x_0}{k+1}\right)^2+\frac{(x_{k+1}-x_0)^2}{k+1}\right)\right)dx_k=$$

$$=\frac{\exp(\frac{mi}{2(k+1)\hbar\epsilon}(x_{k+1}-x_0)^2)}{\sqrt{k+1}}$$

$$G(x,y,t>0)=\sqrt{\frac{m}{2\pi i\hbar\epsilon N}}\exp\left(\frac{mi}{2N\hbar\epsilon}(x_N-x_0)^2\right)$$

$$x_0=x,\quad x_N=y,\quad N\epsilon=T$$

$$G(x,y,t>0)=\sqrt{\frac{m}{2\pi i\hbar T}}\exp\left(\frac{im(y-x)^2}{2\hbar T}\right)$$

ПТФ-16.з2. Частица в магнитном поле (50 б).

Вычислите пропагатор квантовой частицы, движущийся в плоскости в постоянном магнитном поле B, перпендикулярном этой плоскости ($\mathbf{r}(t)=(x(t),y(t))$):

$$G(\mathbf{R}_1,\mathbf{R}_2,T)=\int\limits_{\mathbf{r}(0)=\mathbf{R}_1}^{\mathbf{r}(T)=\mathbf{R}_2}\mathcal{D}[\mathbf{r}(t)]\exp\left(\frac{i}{2\hbar}\int\limits_0^T\left(m(\dot{x}^2+\dot{y}^2)+\frac{e}{c}B(x\dot{y}-y\dot{x})\right)dt\right)$$

(сперва убедившись, что данное действие действительно описывает именно эту систему). Используя функцию Грина, найдите спектр соответствующей квантовой задачи (решение которой, напомним, даётся макроскопически вырожденными *уровнями Ландау*).
Подсказка: хотя этот интеграл можно вычислить и непосредственно, может оказаться удобным переход во вращающуюся систему отсчёта – провести следующую замену в функциональном интеграле:

$$\begin{cases}x'(t)=x(t)\cos\Omega t+y(t)\sin\Omega t,\\ y'(t)=-x(t)\sin\Omega t+y(t)\cos\Omega t\end{cases}$$

и при правильном выборе частоты Ω задача значительно упрощается. Не забудьте о модификации граничных условий из-за такой замены!

Solution

Сделаем замену:

$$\begin{cases} x'(t) = x(t)\cos\Omega t + y(t)\sin\Omega t, \\ y'(t) = -x(t)\sin\Omega t + y(t)\cos\Omega t \end{cases}$$

Обратная замена:

$$\begin{cases} x(t) = x'(t)\cos\Omega t - y'(t)\sin\Omega t, \\ y(t) = x'(t)\sin\Omega t + y'(t)\cos\Omega t \end{cases}$$

$$\begin{cases} \dot{x}(t) = (\dot{x}'(t) - \Omega y'[t])\cos\Omega t - (\dot{y}'(t) + \Omega x'(t))\sin\Omega t, \\ \dot{y}(t) = (\dot{x}'(t) - \Omega y'[t])\sin\Omega t + (\dot{y}'(t) + \Omega x'(t))\cos\Omega t \end{cases}$$

$$\dot{x}^2(t) + \dot{y}^2(t) = \dot{x}'^2(t) + \dot{y}'^2(t) + \Omega^2(x'^2(t) + y'^2(t)) + 2\Omega(x'(t)\dot{y}'(t) - y'(t)\dot{x}'(t))$$

$$x(t)\dot{y}(t) - y(t)\dot{x}(t) = \Omega(x'^2(t) + y'^2(t)) + x'(t)\dot{y}'(t) - \dot{x}'(t)y'(t)$$

$$m(\dot{x}^2 + \dot{y}^2) + \frac{e}{c}B(x\dot{y} - y\dot{x}) = m(\dot{x}'^2(t) + \dot{y}'^2(t)) + \left(m\Omega^2 + \frac{eB\Omega}{c}\right)(x'^2(t) + y'^2(t)) + \\ + \left(2m\Omega + \frac{eB}{c}\right)(x'(t)\dot{y}'(t) - \dot{x}'(t)y'(t))$$

Пусть $\Omega = -\frac{eB}{2mc}$, тогда

$$m(\dot{x}^2 + \dot{y}^2) + \frac{e}{c}B(x\dot{y} - y\dot{x}) = m(\dot{x}'^2(t) + \dot{y}'^2(t)) + \Omega\frac{eB}{2c}(x'^2(t) + y'^2(t)) = m(\dot{x}'^2(t) + \dot{y}'^2(t)) - \\ - \frac{e^2B^2}{4mc^2}(x'^2(t) + y'^2(t))$$

$$G(\mathbf{R}_1, \mathbf{R}_2, T) = \int\limits_{\mathbf{r}'(0)=\mathbf{R}_1}^{\mathbf{r}'(T)=\mathbf{R}_2} \mathcal{D}[\mathbf{r}'(t)] \exp\left(\frac{i}{2\hbar}\int\limits_0^T \left(m(\dot{x}'^2 + \dot{y}'^2) - \frac{e^2B^2}{4mc^2}(x'^2 + y'^2)\right)dt\right)$$

Получился пропагатор с лагранжианом:

$$L = \frac{m(\dot{x}'^2 + \dot{y}'^2)}{2} - \frac{e^2B^2}{8mc^2}(x'^2 + y'^2)$$

Получившийся потенциал $V(\mathbf{r}\,') = \frac{e^2B^2}{8mc^2}(x'^2 + y'^2)$ – гармонический осциллятор в 2D с частотой $\omega = \frac{eB}{2mc} = \Omega$.

$$G(\mathbf{R}_1, \mathbf{R}_2, T) = \int\limits_{\mathbf{r}\,'(0)=\mathbf{R}_1'}^{\mathbf{r}\,'(T)=\mathbf{R}_2'} \mathcal{D}[\mathbf{r}\,'(t)] e^{\frac{iS[\mathbf{r}_{\text{cl}}'(t)]}{\hbar}}$$

$$\int\limits_{\mathbf{r}'(0)=\mathbf{R}_1'}^{\mathbf{r}'(T)=\mathbf{R}_2'} \mathcal{D}[\mathbf{r}'(t)] = \left(\sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}\right)^2 = \frac{m\omega}{2\pi i\hbar\sin\omega T}$$

$$S[\mathbf{r}_{\text{cl}}'(t)] = \frac{m\omega}{2}\frac{(r'^2(0) + r'^2(T))\cos\omega T - 2\mathbf{r}'(0)\cdot\mathbf{r}'(T)}{\sin\omega T}$$

$$r'^2(0) = x^2(0) + y^2(0) = r^2(0) = R_1^2, \quad r'^2(T) = x^2(T) + y^2(T) = r^2(T) = R_2^2$$

$$\mathbf{r}'(0)\cdot\mathbf{r}'(T) = (x(0)x(T) + y(0)y(T))\cos\Omega T + (x(0)y(T) - x(T)y(0))\sin\Omega T = \\ = (R_{1x}R_{2x} + R_{1y}R_{2y})\cos\Omega T + (R_{1x}R_{2y} - R_{2x}R_{1y})\sin\Omega T$$

$$S[\mathbf{r}_{\text{cl}}'(t)] = \frac{m\Omega}{2}((R_1^2 + R_2^2)\operatorname{ctg}\Omega T - 2((R_{1x}R_{2x} + R_{1y}R_{2y})\operatorname{ctg}\Omega T + (R_{1x}R_{2y} - R_{2x}R_{1y})))$$

$$S[\mathbf{r}_{\text{cl}}'(t)] = \frac{m\Omega}{2}(((R_{1x} - R_{2x})^2 + (R_{1y} - R_{2y})^2)\operatorname{ctg}\Omega T - 2(R_{1x}R_{2y} - R_{2x}R_{1y}))$$

$$G(\mathbf{R}_1, \mathbf{R}_2, T) = \frac{m\Omega}{2\pi i\hbar\sin\Omega T}\exp\left(\frac{im\Omega}{2\hbar}(((R_{1x} - R_{2x})^2 + (R_{1y} - R_{2y})^2)\operatorname{ctg}\Omega T - 2(R_{1x}R_{2y} - R_{2x}R_{1y}))\right)$$

$$\frac{1}{2i\sin\omega T} = e^{-i\omega T}\sum_{l=0}^{\infty} e^{-2i\omega lT}, \quad i\cot\omega T = -\frac{1 + e^{-2i\omega T}}{1 - e^{-2i\omega T}} = -\left(1 + e^{-2i\omega T}\right)\sum_{l=0}^{\infty} e^{-2i\omega lT} = -2\sum_{l=0}^{\infty} e^{-2i\omega lT}$$

Уровни энергии:

$$E_{n_x,n_y} = \frac{eB\hbar}{mc}(n_x + n_y + 1), \quad n_x, n_y \in \mathbb{N}_0$$

ПТФ-16.з3. «Мацубаровский» функциональный интеграл (25 б).

Рассмотрите квантовую частицу, описываемую гамильтонианом $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$. Если такая частица находится в равновесии при температуре $T = \beta^{-1}$, её матрица плотности имеет вид $\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}}$, и её статсумма

$$Z = \mathrm{Tr}(e^{-\beta \hat{H}})$$

Используя аналогию между равновесной матрицей плотности и оператором эволюции в мнимом времени $t = -i\tau \Rightarrow \hat{U}(t) = e^{-\hat{H}\tau}$, постройте представление функционального интеграла для статсуммы Z. Покажите, что интегрирование должно проводиться по всем траекториям в мнимом времени $x(\tau)$, которые периодичны в мнимом времени: $x(\tau + \beta) \equiv x(\tau)$. Полученное выражение при этом должно получаться формальной заменой $t = -i\tau$ в исходном выражении (такая формальная замена носит название *Виковского поворота*).

Solution

Запаздывающая функция Грина – аплитуда распространения квантовомеханической частицы из точки $\mathbf{x}$ в точку $\mathbf{y}$ за время β:

$$G^R(\mathbf{x}, \mathbf{y}, \beta) = \langle \mathbf{y} | \hat{U}(\beta) | \mathbf{x} \rangle$$

В гамильтониане импульс и координата разделяются. Разобъём отрезок времени длины β на $N \to \infty$ одинаковых кусочков размера $\epsilon = \frac{\beta}{N} \to 0$ и представим оператор эволюции в виде $\hat{U}(\beta) = \prod\limits_{i=1}^{N} \hat{U}(\epsilon)$. Эволюцию на бесконечно малое время ϵ можно записать в виде $\hat{U}(\epsilon \to 0) = e^{-\hat{H}\epsilon} \approx e^{-\hat{V}\epsilon} e^{-\hat{K}\epsilon}$. Получаем выражение для оператора эволюции в виде произведения $2N$ множителей (удобно каждому приписать своё время $\tau_k = k\epsilon$):

$$\hat{U}(\tau) = e^{-\hat{V}\epsilon} e^{-\hat{K}\epsilon} ... e^{-\hat{V}\epsilon} e^{-\hat{K}\epsilon}$$

Вставим после каждого члена $e^{-\hat{K}\epsilon}$ (при $\tau = \tau_k$) единицу в виде разложения по координатному базису $\mathbb{I} = \int d\mathbf{x}_k |\mathbf{x}_k\rangle\langle\mathbf{x}_k|$, а после членов $e^{-\hat{V}\epsilon}$ – по импульсному $\hat{I} = \int (d\mathbf{p}_k) |\mathbf{p}_k\rangle\langle\mathbf{p}_k|$

$$G^R(\mathbf{x}, \mathbf{y}, \beta) = \int \prod_{k=1}^{N-1} d\mathbf{x}_k \int \prod_{k=1}^{N} (d\mathbf{p}_k) \langle \mathbf{y} | e^{-\hat{V}\epsilon} | \mathbf{p}_N \rangle \langle \mathbf{p}_N | e^{-i\hat{K}\epsilon} | \mathbf{x}_{N-1} \rangle ... \langle \mathbf{x}_1 | e^{-\hat{V}\epsilon} | \mathbf{p}_1 \rangle \langle \mathbf{p}_1 | e^{-i\hat{K}\epsilon} | \mathbf{x} \rangle$$

Поскольку операторы $e^{-\hat{V}\epsilon}$ – собственные для координаты, а $e^{-\hat{K}\epsilon}$ – для импульса, то блоки вычисляются:

$$\langle \mathbf{x}_k | e^{-\hat{V}\epsilon} | \mathbf{p}_k \rangle \langle \mathbf{p}_k | e^{-\hat{K}\epsilon} | \mathbf{x}_{k-1} \rangle = e^{-V(\mathbf{x}_k)\epsilon} e^{i\mathbf{p}_k \mathbf{x}_k} e^{-K(\mathbf{p}_k)\epsilon} e^{-i\mathbf{p}_k \mathbf{x}_{k-1}}$$

$$G^R(\mathbf{x}, \mathbf{y}, \beta) = \int \prod_{k=1}^{N-1} d\mathbf{x}_k \int \prod_{k=1}^{N} (d\mathbf{p}_k) \exp\left(\epsilon \sum_{k=1}^{N} \left(i\mathbf{p}_k \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\epsilon} - \hat{H}(\mathbf{x}_k, \mathbf{p}_k) \right) \right)$$

Возьмём интеграл по импульсам. Кинетическая энергия $K(p) = \frac{p^2}{2m}$, поэтому

$$\int (d\mathbf{p}_k) \exp\left(\epsilon \sum_{k=1}^{N} \left(i\mathbf{p}_k \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\epsilon} - \frac{\mathbf{p}_k^2}{2m} \right) \right) = \left(\frac{m}{2\pi\epsilon} \right)^{\frac{d}{2}} \exp\left(-\epsilon \frac{m}{2} \left(\frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\epsilon} \right)^2 \right)$$

$$G^R(\mathbf{x}, \mathbf{y}, \beta) = \left(\frac{m}{2\pi\epsilon} \right)^{\frac{Nd}{2}} \int \prod_{k=1}^{N-1} d\mathbf{x}_k \exp\left(-\epsilon \sum_{k=1}^{N} \left(\frac{m}{2} \left(\frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\epsilon} \right)^2 + V(\mathbf{x}_k) \right) \right)$$

В экспоненте стоит конечная аппроксимация интеграла:

$$\sum_{k=1}^{N} \epsilon \left(\frac{m}{2} \left(\frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\epsilon} \right)^2 + V(\mathbf{x}_k) \right) \approx \int_0^\beta d\tau \left(\frac{m}{2} \dot{\mathbf{x}}(\tau)^2 + V(\mathbf{x}(\tau)) \right)$$

Выберем меру интегрирования:

$$\mathcal{D}[\mathbf{x}(t)] = \left(\frac{m}{2\pi\epsilon} \right)^{\frac{Nd}{2}} \prod_{k=1}^{N-1} d\mathbf{x}_k$$

$$G^R(\mathbf{x},\mathbf{y},\beta)=\int\limits_{\mathbf{x}(0)=\mathbf{x}}^{\mathbf{x}(\beta)=\mathbf{y}}\mathcal{D}[\mathbf{x}(t)]\exp\left(-\int\limits_0^\beta d\tau\left(\frac{m}{2}\dot{\mathbf{x}}(\tau)^2+V(\mathbf{x}(\tau)\right)\right)$$

Матрица плотности в координатном представлении:

$$\rho(\mathbf{x},\mathbf{y},\beta)=\langle\mathbf{y}|\hat{\rho}|\mathbf{x}\rangle=\int\limits_{\mathbf{x}(0)=\mathbf{x}}^{\mathbf{x}(\beta)=\mathbf{y}}\mathcal{D}[\mathbf{x}(t)]\exp\left(-\int\limits_0^\beta d\tau\left(\frac{m}{2}\dot{\mathbf{x}}(\tau)^2+V(\mathbf{x}(\tau)\right)\right)$$

Статистическая сумма:

$$Z=\mathrm{Tr}\rho(\mathbf{x},\mathbf{y},\beta)=\int d\mathbf{x}\rho(\mathbf{x},\mathbf{x},\beta)=\int d\mathbf{x}\int\limits_{\mathbf{x}(0)=\mathbf{x}}^{\mathbf{x}(\beta)=\mathbf{x}}\mathcal{D}[\mathbf{x}(t)]\exp\left(-\int\limits_0^\beta d\tau\left(\frac{m}{2}\dot{\mathbf{x}}(\tau)^2+V(\mathbf{x}(\tau)\right)\right)$$

Как видно, интегрирование идёт по периодическим траекториям $x(\tau)=x(\tau+\beta)$. Заметим, что полученное выражение получается из исходного при помощи Виковского поворота $t=-i\tau$.

20.2.3 Problems about Instantons and Tunneling

ПТФ-17.y1 Квазиклассика и инстантоны (30 б).

Для двухъямного потенциала, что разбирался на семинаре (???), вычислите расщепление уровней в квазиклассическом приближении. Насколько квазиклассическое приближение отличается от правильного ответа, даваемого инстантонным вычислением?

Указание: стандартная формула в квазиклассическом приближении гарантирует правильный численный фактор в предэкспоненте; поэтому именно с такой точностью необходимо вычислить и квазиклассическое действие. Обратите внимание, что действие необходимо считать на энергии, отличной от минимума в соответствующей яме; поправка от этого отличия существенна, поскольку она стоит в экспоненте, и имеется серия неравенств $S(0)\gg|S(E)-S(0)|\gg1$. Несложно убедиться, что эта поправка логарифмическая; причём **вычисление необходимо проводить с точностью до числа под логарифмом** (поскольку это число в конечном итоге модифицирует численный префактор в конечном ответе!).

Сделать это можно следующим образом. Во-первых, технически чуть проще вычислять не само действие $S(E)$, а его производную $\partial S/\partial E$, которая логарифмически расходится при $E\to0$. Для вычисления численного фактора под логарифмом, предлагается ввести произвольный промежуточный пространственный масштаб Λ, удовлетворяющий серии неравенств $|x_1+\eta|\ll\Lambda\ll\eta$ (где x_1 – положение левой точки остановки, которая близка к минимуму $-\eta$), и разбить интеграл на два интервала $\int\limits_{x_1}^{\Lambda}+\int\limits_{\Lambda}^{0}$. В первом интеграле первое же неравенство позволяет использовать осцилляторное приближение для потенциала; а во втором интеграле второе неравенство позволяет использовать разложение в ряд Тейлора по энергии. После соответствующих вычислений (с необходимой точностью!), промежуточный масштаб Λ, в силу своей произвольности, из ответа должен сократиться.

Solution

Гамильтониан:

$$\hat{H}=-\frac{1}{2}\partial_x^2+\lambda(x^2-\eta^2)^2$$

Действие в квазиклассическим приближении:

$$S=2\sqrt{2}\int\limits_{-\eta+\delta\eta}^{0}\sqrt{\lambda(x^2-\eta^2)^2-E}dx,\quad E=4\lambda\eta^2\delta\eta^2$$

Разобьём пределы интегрирования на 2:

$$S=2\sqrt{2}\int\limits_{-\eta+\delta\eta}^{-\eta+\Lambda}\sqrt{\lambda(x^2-\eta^2)^2-E}dx+2\sqrt{2}\int\limits_{-\eta+\Lambda}^{0}\sqrt{\lambda(x^2-\eta^2)^2-E}dx=$$

$$=2\sqrt{2}\int\limits_{\delta\eta}^{\Lambda}\sqrt{4\lambda\eta^2y^2-E}dy+2\sqrt{2}\int\limits_{-\eta+\Lambda}^{0}\sqrt{\lambda(x^2-\eta^2)^2-E}dx$$

В 1 интеграле (S_1) работает осцилляторное приближение, поскольку $\Lambda \ll \eta$. Вычислим его, воспользовавшись уазанием:

$$\frac{\partial S_1}{\partial E} = -2\sqrt{2}\int\limits_{\delta\eta}^{\Lambda} \frac{dy}{2\sqrt{4\lambda\eta^2 y^2 - E}} = -\frac{\sqrt{2}}{2\sqrt{\lambda}\eta}\int\limits_{1}^{\frac{\Lambda}{\delta\eta}} \frac{dz}{\sqrt{z^2-1}} = -\frac{\sqrt{2}}{2\sqrt{\lambda}\eta}\log\left(\frac{\Lambda}{\delta\eta} + \sqrt{\left(\frac{\Lambda}{\delta\eta}\right)^2 - 1}\right)$$

$$S_1 = -\frac{\sqrt{2}}{2\sqrt{\lambda}\eta}\int \log\left(\frac{\Lambda}{\delta\eta} + \sqrt{\left(\frac{\Lambda}{\delta\eta}\right)^2 - 1}\right) dE, \quad dE = 8\lambda\eta^2\delta\eta d(\delta\eta)$$

$$S_1 = -4\sqrt{2\lambda}\eta\int\limits_0^{\delta\eta} \delta\eta \log\left(\frac{\Lambda}{\delta\eta} + \sqrt{\left(\frac{\Lambda}{\delta\eta}\right)^2 - 1}\right) d(\delta\eta) = -2\sqrt{2\lambda}\eta\left(\Lambda(\Lambda - \sqrt{\Lambda^2 - (d\eta)^2}) + \right.$$
$$\left. + (\delta\eta)^2 \log\left(\frac{\Lambda}{\delta\eta} + \sqrt{\left(\frac{\Lambda}{\delta\eta}\right)^2 - 1}\right)\right) \approx 2\sqrt{2\lambda}\eta^2 - \sqrt{2\lambda}\eta(\delta\eta)^2\left(1 + 2\log\left(\frac{2\Lambda}{\delta\eta}\right)\right)$$

Во 2 интеграле (S_2) будет раскладывать в ряд по степеням $\frac{E}{\lambda(\eta^2 - x^2)^2}$.

$$S_2 = 2\sqrt{2}\int\limits_{-\eta+\Lambda}^{0} \sqrt{\lambda(x^2-\eta^2)^2 - E}dx \approx 2\sqrt{2\lambda}\int\limits_{-\eta+\Lambda}^{0} |x^2-\eta^2|\left(1 - \frac{E}{4(\eta^2-x^2)^2}\right)dx =$$
$$= 2\sqrt{2\lambda}\left(\eta^2(\Lambda-\eta) - \frac{(\Lambda-\eta)^3}{3} - \frac{E\sqrt{\lambda}}{2}\int\limits_{-\eta+\Lambda}^{0}\frac{dx}{\lambda(\eta^2-x^2)}\right) =$$
$$= 2\sqrt{2\lambda}\left(\frac{2}{3}\eta^3 - \eta\Lambda^2 + \frac{\Lambda^3}{3} - \frac{E\log\left(-1+\frac{2\eta}{\Lambda}\right)}{4\eta\lambda}\right) = 2\sqrt{2\lambda}\left(\frac{2}{3}\eta^3 - \eta\Lambda^2 + \frac{\Lambda^3}{3}\right) -$$
$$- \frac{E\sqrt{2}\left(\log\left(\frac{2\eta}{\Lambda}\right) - \frac{\Lambda}{2\eta}\right)}{2\eta\sqrt{\lambda}} = 2\sqrt{2\lambda}\left(\frac{2\eta^3}{3} - \eta\Lambda^2 + \frac{\Lambda^3}{3} - \eta(\delta\eta)^2\left(\log\left(\frac{2\eta}{\Lambda}\right) - \frac{\Lambda}{2\eta}\right)\right)$$

$$S = S_1 + S_2 = \frac{2}{3}\omega\eta^2 - \log\left(\frac{4\eta}{\delta\eta}\right) - \frac{1}{2}, \quad \omega = 8\lambda\eta^2(\delta\eta)^2$$

Расщепление уровней:

$$E = \frac{\omega}{2} \pm \frac{\omega}{2\pi}e^{-S} = \frac{\omega}{2} \pm \frac{\omega}{2\pi}e^{-S} = \frac{\omega}{2} \pm \frac{\omega}{2\pi}\exp\left(-\frac{2\omega\eta^2}{3}\right)\frac{4\eta}{\delta\eta}e^{\frac{1}{2}}$$

$$\Delta = \frac{2\sqrt{e}}{\pi}\omega^{\frac{3}{2}}\eta e^{-\frac{2\omega\eta^2}{3}}$$

Ответ отличается от инстантонного в $\sqrt{\frac{e}{\pi}}$ раз.

ПТФ-17.з1. Инстантоны и “математический маятник” (70 б).

Рассмотрите движение частицы массы $m = 1$ в периодическом потенциале $U(x) = \lambda(1 - \cos\frac{x}{\eta})$. Вычислите одноинстантонный вклад в амплитуду перехода между двумя минимумами $0 \to 2\pi\eta$ за большое мнимое время β – Евклидову функцию Грина $G_E(2\pi\eta, 0, \beta)$.

• **(5 б)** Найдите инстантонную траекторию, соответствующую такому переходу, вычислите действие на ней. Вычислите явно оператор, определяющий квадратичные флуктуации в окрестности инстантона.

• **(10 б)** Исследуйте спектр полученного оператора. Вычислите фазовые сдвиги непрерывного спектра и уровни энергии связанных состояний.

• **(10 б)** Рассмотрите отнормированный на осциллятор пропагатор. Идентифицируйте нулевую моду, выполните интегрирование по ней.

• **(35 б)** Вычислите вклад в отношение определителей от дискретного и непрерывного спектра.

• **(10 б)** Просуммируйте инстантонный газ для искомой амплитуды перехода. Сравнив полученный ответ с ответом для соответствующей модели сильной связи, извлеките из полученного ответа ширину зоны непрерывного спектра соответствующей квантомеханической задачи.

Solution

• Потенциал имеет минимумы в точках $x = 2\pi\eta n, n \in \mathbb{Z}$, вблизи которых он имеет осцилляторное разложение $U(x) = \frac{1}{2}\omega^2 x^2$ с частотами $\omega^2 = \frac{\lambda}{\eta^2}$. Евклидово действие:

$$S_E[x(\tau)] = \int \left(\frac{1}{2}(\partial_\tau x)^2 + U(x(\tau))\right) d\tau$$

Нужно найти экстремум действия с граничными условиями $x(\tau \to -\infty) = 0$, $x(\tau \to \infty) = 2\pi\eta$.

$$\frac{\delta S_E}{\delta x(\tau)} = 0 \to \partial_\tau^2 x = U'(x(\tau))$$

Закон сохранения энергии:

$$E = \frac{1}{2}(\partial_\tau x)^2 - U(x(\tau)) = \text{const}$$

На нашей траектории $E = 0$, поэтому

$$\frac{1}{2}(\partial_\tau x)^2 = U(x(\tau)) \to \frac{dx}{\sqrt{1 - \cos\frac{x}{\eta}}} = \sqrt{2\lambda} d\tau$$

$$\sqrt{2}\eta \ln\left(\tan\frac{x}{4\eta}\right) = \sqrt{2\lambda}\tau \to x_{\text{cl}}(\tau) = 4\eta \arctan\left(e^{\omega\tau}\right)$$

Действие на инстантоне:

$$S_0 = S_E[x_{\text{cl}}(\tau)] = \int\limits_{-\infty}^{\infty} (\partial_\tau x_{\text{cl}})^2 d\tau = \int\limits_{-\infty}^{\infty} \frac{4\lambda}{\cosh^2\left(\frac{\sqrt{\lambda}\tau}{\eta}\right)} d\tau$$

$$S_0 = 8\eta\sqrt{\lambda} = 8\eta^2\omega$$

Квадратичное разложение вблизи потенциала:

$$S_E[x_{\text{cl}}(\tau) + z(\tau)] \approx S_0 + \frac{1}{2}\int\limits_0^\beta d\tau((\partial_\tau z)^2 + U''(x_{\text{cl}}(\tau))z^2(\tau))$$

$$U''(x_{\text{cl}}(\tau)) = \frac{\lambda}{\eta^2}\cos\frac{x_{\text{cl}}}{\eta} = \omega^2\cos\left(4\arctan\left(e^{\omega\tau}\right)\right)$$

В квадратичном разложении действия стоит линейный оператор:

$$\hat{L} = -\partial_\tau^2 + U''(x_{\text{cl}}(\tau)) = -\partial_\tau^2 + \omega^2\cos\left(4\arctan\left(e^{\omega\tau}\right)\right)$$

$$\hat{L} = -\partial_\tau^2 + \omega^2\left(1 - \frac{2}{\cosh^2\omega\tau}\right)$$

• Уравнение на спектр оператора $\hat{L}$:

$$\left(-\partial_\tau^2 - \frac{2\omega^2}{\cosh^2\omega\tau}\right)\psi_n(\tau) = (\epsilon_n - \omega^2)\psi_n(\tau)$$

Данное уравнение – уравнение Шрёдингера в потенциале $\frac{1}{\cosh^2 x}$, которое было разобрано в семинаре 4. Воспользуемся ответами из того семинара, в которые нужно подставить следующие значения параметров:

$$m = \frac{1}{2}, \quad a = \frac{1}{\omega}, \quad U_0 = 2\omega^2$$

$$u = \frac{U_0}{1/2ma^2} = 2, \quad s = \frac{1}{2}(\sqrt{1+4u} - 1) = 1$$

Энергии связанных состояний:

$$E_n = -\frac{(s-n)^2}{2ma^2} = -\omega^2(s-n)^2 \to E_0 = -\omega^2$$

$$\epsilon_0 = E_0 + \omega^2 = 0$$

Волноваяя функция нулевой моды:

$$\psi_0(\tau) = \frac{C_0}{\cosh \omega\tau}$$

При целом $s = 1$ рассеяние оказывается безотражательным. Непрерывный спектр характеризуется волновым вектором k, так что энергия $E_k = \frac{k^2}{2m} = k^2 \to \epsilon_k = \omega^2 + k^2$. Волновые функции:

$$\psi_k(x) \approx \begin{cases} \frac{\Gamma(1-ika)\Gamma(-ika)}{\Gamma(-ika-1)\Gamma(-ika+2)} e^{ikx} \equiv e^{ikx+i\delta(k)}, & x \to -\infty \\ e^{ikx}, & x \to +\infty \end{cases}$$

$$e^{-i\delta(k)} = \frac{\Gamma(-ika-1)\Gamma(-ika+2)}{\Gamma(1-ika)\Gamma(-ika)} = \frac{1-ika}{-1-ika} = -\frac{1-ika}{1+ika} = e^{-i\pi - 2i\arctan ka}$$

$$\delta(k) = 2\arctan ka - \pi = \begin{cases} \pi, & k = 0 \\ 0, & k \to \infty \end{cases}$$

Дискретизация непрерывного спектра. Волновая функция имеет вид $\psi_n(x) = A\psi_k(x) + B\psi_k^*(x)$, тогда граничные условия:

$$\begin{cases} A\psi_k(0) + B\psi_k^*(0) = 0, \\ A\psi_k(\beta) + B\psi_k^*(\beta) = 0 \end{cases}$$

Условие совместности системы:

$$\det \begin{pmatrix} \psi_k(0) & \psi_k^*(0) \\ \psi_k(\beta) & \psi_k^*(\beta) \end{pmatrix} = 0$$

Подставляем асимптотики:

$$\det \begin{pmatrix} 1 & 1 \\ e^{ik\beta - i\delta(k)} & e^{-ik\beta + i\delta(k)} \end{pmatrix} = 0 \to k_n\beta - \delta(k_n) = \pi n$$

Решим трансцендентное уравнение по теории возмущений:

$$k_n^{(0)} \approx p_n = \frac{\pi n}{\beta} \to k_n^{(1)} \approx p_n + \frac{\delta(p_n)}{\beta}$$

- Функция Грина гармонического осциллятора:

$$G_0(\beta) = \int\limits_{z(0)=0}^{z(\beta)=0} \mathcal{D}[z(\tau)] \exp\left(-\frac{1}{2}\int\limits_0^\beta ((\partial_\tau z)^2 + \omega^2 z^2)\right)$$

Отношение функций Грина:

$$\frac{G(2\pi\eta, 0, \beta)}{G_0(\beta)} = e^{-S_0} \frac{\int\limits_{z(0)=0}^{z(\beta)=0} \mathcal{D}[z(\tau)] \exp\left(-\frac{1}{2}\int\limits_0^\beta d\tau((\partial_\tau z)^2 + U''(x_{\text{cl}}(\tau))z^2(\tau))\right)}{\int\limits_{z(0)=0}^{z(\beta)=0} \mathcal{D}[z(\tau)] \exp\left(-\frac{1}{2}\int\limits_0^\beta d\tau((\partial_\tau z)^2 + \omega^2 z^2(\tau))\right)}$$

Спектр гармонического осциллятора:

$$\epsilon_p^{(0)} = \omega^2 + p^2, \quad p = p_n = \frac{\pi n}{\beta}$$

Разложене в числителе $z(\tau) = \sum\limits_n c_n\psi_n(\tau)$ и в знаменателе $z(\tau) = \sum\limits_n c_n\psi_n^{(0)}(\tau)$. Интеграл по нулевой моде:

$$\int dc_0 = \int d\tau_c \frac{dc_0}{d\tau_c} = \sqrt{S_0}\beta$$

$$\int dc_1 e^{-\frac{1}{2}\epsilon_1^{(0)} c_1^2} = \sqrt{\frac{2\pi}{\epsilon_1^{(0)}}} = \sqrt{\frac{2\pi}{\omega^2 + \frac{\pi^2}{\beta^2}}} \approx \frac{\sqrt{2\pi}}{\omega}$$

$$\frac{G(2\pi\eta, 0, \beta)}{G_0(\beta)} = e^{-S_0}\omega\beta\sqrt{\frac{S_0}{2\pi}} \left(\frac{\det'(-\partial_\tau^2 + U''(x_{\rm cl}(\tau)))}{\det'(-\partial_\tau^2 + \omega^2)}\right)^{-\frac{1}{2}}$$

$$\frac{\det'}{\det'} = \prod_{n=1}^{\infty} \frac{\omega^2 + k_n^2}{\omega^2 + p_{n+1}^2} = \exp\left(\sum_{n=1}^{\infty} \log \frac{\omega^2 + k_n^2}{\omega^2 + p_{n+1}^2}\right) = \exp\left(\sum_{n=1}^{\infty} \log\left(1 + \frac{k_n^2 - p_{n+1}^2}{\omega^2 + p_{n+1}^2}\right)\right) \approx$$
$$\approx \exp\left(\sum_{n=1}^{\infty} \frac{2p_{n+1}(k_n - p_{n+1})}{\omega^2 + p_{n+1}^2}\right) = \exp\left(\frac{1}{\beta}\sum_{n=1}^{\infty} \frac{2p_{n+1}(\delta(p_n) - \pi)}{\omega^2 + p_{n+1}^2}\right)$$

Для суммирования плавной функции заменим сумму на интеграл $\sum\limits_n = \int\limits_0^\infty \frac{\beta dp}{\pi}$:

$$\frac{\det'}{\det'} = \exp\left(\int_0^\infty \frac{dp 2p(\delta(p) - \pi)}{\pi(\omega^2 + p^2)}\right) = \exp\left(-\frac{1}{\pi}\int_0^\infty dp \frac{d\delta}{dp} \log\frac{\omega^2 + p^2}{\omega^2}\right)$$

$$\frac{\det'}{\det'} = \frac{1}{4}$$

Одноинстантонный ответ:

$$\frac{G(2\pi\eta, 0, \beta)}{G_0(\beta)} = e^{-S_0}\omega\beta\sqrt{\frac{S_0}{2\pi}}\sqrt{4} = \sqrt{\frac{S_0}{\pi}}\omega\beta e^{-S_0} = \sqrt{\frac{8\eta^2\omega}{\pi}}\omega\beta e^{-8\eta^2\omega}$$

• В случае n инстантонов вклад $S_n = nS_0$, полная фаза рассеяния $\delta^{(n)}(p) = n\delta(p)$. С каждым из инстантонов связана нулевая мода

$$\int\limits_{0<\tau_1<\ldots<\tau_n<\beta} d\tau_1 \ldots d\tau_n = \frac{\beta^n}{n!}$$

Для перехода $0 \to 2\pi\eta$ только конфигурации с нечётным количеством интсантонов дают вклад.

$$\frac{G(2\pi\eta, 0, \beta)}{G_0(\beta)} = \sum_{n=0}^{\infty} \frac{^n_{2n+1}}{(2n+1)!} \left(\sqrt{\frac{8\eta^2\omega}{\pi}}\omega\beta e^{-8\eta^2\omega}\right)^{2n+1}$$

ПТФ-18.у1 «Математический маятник», продолжение (10 б).

Вычислите функциональный детерминант, возникающий при исследовании задачи из предыдущего семинара, и сравните его с полученным непосредственным вычислением.

Solution

ПТФ-18.з1. Модификации Гельфанда-Яглома (50 б)

Покажите, как нужно модифицировать теорему Гельфанда-Яглома для вычисления следующих определителей типа уравнения Шрёдингера:

(30 б) Одномерный оператор $\hat{H} = -\partial_x^2 + U(x)$, но для случая периодических граничных условий $\psi(x) \equiv \psi(x + L)$. Вычислите отношение определителей $\frac{\det(-\partial_x^2 + k_1^2)}{\det(-\partial_x^2 + k_2^2)}$.

(10 б) Двумерный оператор $\hat{H} = -\nabla^2 + U(r)$ для сферически-симметричного потенциала.

(10 б) Аналогично, трёхмерный случай.

Solution

•
• Двумерный оператор:

$$\hat{H} = -\nabla^2 + U(r) = -\partial_r^2 - \frac{1}{r}\partial_r - \frac{1}{r^2}\partial_\varphi^2 + U(r)$$

Уравнение на собственные значения:

$$\hat{H}\psi = \lambda\psi$$

Сведём уравнение к одномерному. Разложим волновую функцию по базису $\psi(r,\varphi) = \sum\limits_{m=-\infty}^{\infty} f_m(r)e^{im\varphi}$ и получим

$$-\partial_r^2 f_m(r) - \frac{1}{r}\partial_r f_m(r) + \left(\frac{m^2}{r^2} + U(r) - \lambda\right) f_m(r) = 0$$

Модификация Гельфанда-Яглома для двумерного сферически-симметричного потенциала:

$$\frac{\det(\hat{H}_1 - \lambda)}{\det(\hat{H}_2 - \lambda)} = \prod_{m=-\infty}^{\infty} \frac{f_m^1(R|\lambda)}{f_m^2(R|\lambda)} = \frac{f_0^1(R|\lambda)}{f_0^2(R|\lambda)} \prod_{m=1}^{\infty} \left(\frac{f_m^1(R|\lambda)}{f_m^2(R|\lambda)}\right)^2$$

где $f_m^{1,2}(r|\lambda)$ – решения задачи

$$-\partial_r^2 f_m^{1,2}(r|\lambda) - \frac{1}{r}\partial_r f_m^{1,2}(r|\lambda) + \left(\frac{m^2}{r^2} + U_{1,2}(r) - \lambda\right) f_m^{1,2}(r|\lambda) = 0$$

с граничными условиями $f_m^{1,2}(0|\lambda) = 0$, $\partial_r f_m^{1,2}(0|\lambda) = 1$.

• Трёхмерный оператор:

$$\hat{H} = -\nabla^2 + U(r)$$

Уравнение на собственные значения:

$$\hat{H}\psi = \lambda\psi$$

Сведём уравнение к одномерному. Разложим волновую функцию по базису $\psi(r,\theta,\varphi) = \sum\limits_{l=0}^{\infty}\sum\limits_{m=-l}^{l} R_l(r)Y_{l,m}(\theta,\varphi)$ и получим

$$-\partial_r^2 R_l(r) - \frac{2}{r}\partial_r R_l + \left(\frac{l(l+1)}{r^2} + U(r) - \lambda\right) R_l(r) = 0$$

Модификация Гельфанда-Яглома для трёхмерного сферически-симметричного потенциала:

$$\frac{\det(\hat{H}_1 - \lambda)}{\det(\hat{H}_2 - \lambda)} = \prod_{l=0}^{\infty}\prod_{m=-l}^{l} \frac{R_l^1(R|\lambda)}{R_l^2(R|\lambda)} = \prod_{l=0}^{\infty} \left(\frac{R_l^1(R|\lambda)}{R_l^2(R|\lambda)}\right)^{2l+1}$$

где $R_l^{1,2}(r|\lambda)$ – решения задачи

$$-\partial_r^2 R_l^{1,2}(r) - \frac{2}{r}\partial_r R_l^{1,2} + \left(\frac{l(l+1)}{r^2} + U_{1,2}(r) - \lambda\right) R_l^{1,2}(r) = 0$$

с граничными условиями $R_l^{1,2}(0|\lambda) = 0$, $\partial_r R_l^{1,2}(0|\lambda) = 1$.

ПТФ-18.з2. Дзета-функция Бесселя? (40 б)

• Вычислите следующее бесконечное произведение, в котором $\mu_n^{(m)}$ – n-тый нуль m-той функции Бесселя $J_m(z)$ (очевидным образом $J_{m>0}(0) = 0$; и этот тривиальный нуль в произведении не участвует):

$$P_m(R) = \prod_{n=1}^{\infty} \frac{1 + (\mu_n^{(m)}/R)^2}{(\mu_n^{(m)}/R)^2}$$

Для этого найдите операторы, которые дают соответствующие собственные числа, а затем вычислите их отношения, используя теорему Гельфанда-Яглома.

• Пусть λ_n – все собственные числа эрмитового оператора $\hat{H}$. Покажите, что дзета-функцию оператора $\hat{H}$, которую мы определим следующим образом:

$$\zeta_H(s) = \sum_{n=0} \frac{1}{\lambda_n^s}$$

для натурального аргумента $s \in \mathbb{N}$ можно сосчитать следующим образом:

$$\zeta_H(s) = \frac{(-1)^{s-1}}{(s-1)!} \frac{\partial^s}{\partial \lambda^s} \left(\log \frac{\det(\hat{H} + \lambda)}{\det \hat{H}} \right) \Big|_{\lambda=0}$$

• Докажите следующие равенства:

$$\sum_{n=1}^{\infty} \frac{1}{(\mu_n^{(0)})^2} = \frac{1}{4}, \quad \sum_{n=1}^{\infty} \frac{1}{(\mu_n^{(0)})^4} = \frac{1}{32}, \quad \sum_{n=1}^{\infty} \frac{1}{(\mu_n^{(1)})^2} = \frac{1}{8}$$

Solution

• Рассмотрим гамильтониан:

$$\hat{H}_m = -\partial_r^2 - \frac{1}{r}\partial_r + \frac{m^2}{r^2}$$

Уравнение на собственные значения:

$$\hat{H}_m \psi_m = \lambda \psi_m, \quad \psi_m(0) = \psi_m(R) = 0$$

$$-\partial_r^2 \psi_m - \frac{1}{r}\partial_r \psi_m + \frac{m^2}{r^2}\psi_m = \lambda \psi_m$$

Пусть $z = \sqrt{\lambda} r$ и $f(z) = \psi(z(r))$, тогда

$$z^2 \partial_z^2 f_m + z \partial_z f_m + (z^2 - m^2) f_m = 0$$

Получилась функция Бесселя (функция Неймана сингулярна в 0):

$$f_m(r|\lambda_m) = C_1 J_m(z) \to \psi_m(r|\lambda_m) = C_1 J_m(\sqrt{\lambda_m} r)$$

$$\psi_m(0|\lambda) = 0, \quad \psi_m(R|\lambda) = 0 \to \sqrt{\lambda_n} R = \mu_n^{(m)}$$

$$\lambda_n = \frac{(\mu_n^{(m)})^2}{R^2}$$

$$P_m(R) = \prod_{n=1}^{\infty} \frac{1 + (\mu_n^{(m)}/R)^2}{(\mu_n^{(m)}/R)^2} = \frac{\det(\hat{H}_m + 1)}{\det(\hat{H}_m)}$$

По теореме Гельфанда-Яглома:

$$P_m(R) = \frac{\det(\hat{H}_m + 1)}{\det(\hat{H}_m)} = \frac{\psi_m^{(1)}(R|\lambda_0)}{\psi_m(R|\lambda_0)}, \quad \lambda_0 \to 0$$

где $\psi_m(r|\lambda_0) = C J_m(\sqrt{\lambda_0} r)$, а $\psi_m^{(1)}(r|\lambda_0)$ – решение задачи

$$-\partial_r^2 \psi_m^{(1)} - \frac{1}{r}\partial_r \psi_m^{(1)} + \frac{m^2}{r^2}\psi_m^{(1)} + \psi_m^{(1)} = \lambda_0 \psi_m^{(1)}$$

Пусть $z = \sqrt{1 - \lambda_0} r$ и $f^{(1)}(z) = \psi^{(1)}(z(r))$, тогда

$$z^2 \partial_z^2 f_m^{(1)} + z \partial_z f_m^{(1)} - (z^2 + m^2) f_m^{(1)} = 0$$

Получилась функция Инфильда (функция Макдональда сингулярна в 0):

$$\psi_m^{(1)}(r|\lambda_0) = C_2 I_m(\sqrt{1 - \lambda_0} r)$$

Асимптотики функций Бесселя и Инфильда:

$$\begin{cases} J_m(\sqrt{\lambda_0}r) \approx \frac{1}{m!}\left(\frac{\sqrt{\lambda_0}r}{2}\right)^m \\ I_m(\sqrt{1-\lambda_0}r) \approx \frac{1}{m!}\left(\frac{\sqrt{1-\lambda_0}r}{2}\right)^m \end{cases}, \quad r \to 0$$

Для того, чтобы $\psi_m^{(1)}(r) \sim \psi_m(r)$, выберем $\frac{C_2}{C_1} = \left(\frac{\lambda_0}{1-\lambda_0}\right)^{\frac{m}{2}}$.

$$P_m(R) = \lim_{\lambda_0 \to 0}\left(\frac{\lambda_0}{1-\lambda_0}\right)^{\frac{m}{2}} \frac{I_m(\sqrt{1-\lambda_0}R)}{J_m(\sqrt{\lambda_0}R)} = \frac{I_m(R)2^m m!}{R^m}$$

$$P_m(R) = \frac{2^m m!}{R^m} I_m(R)$$

$$\frac{\det(\hat{H}+\lambda)}{\det \hat{H}} = \prod_{n=0}^{\infty}\frac{\lambda_n+\lambda}{\lambda_n} = \prod_{n=0}^{\infty}\left(1+\frac{\lambda}{\lambda_n}\right)$$

$$\log\left(\frac{\det(\hat{H}+\lambda)}{\det \hat{H}}\right) = \sum_{n=0}^{\infty}\log\left(1+\frac{\lambda}{\lambda_n}\right) = \sum_{n=0}^{\infty}\sum_{k=1}^{\infty}\frac{(-1)^{k-1}}{k}\left(\frac{\lambda}{\lambda_n}\right)^k$$

$$\frac{\partial^s}{\partial\lambda^s}\left(\log\left(\frac{\det(\hat{H}+\lambda)}{\det \hat{H}}\right)\right)\Big|_{\lambda=0} = \sum_{n=0}^{\infty}\sum_{k=s}^{\infty}\frac{(-1)^{k-1}}{k}\frac{\lambda^{k-s}}{\lambda_n^k}\prod_{m=0}^{s-1}(k-m)\Big|_{\lambda=0} =$$

$$= \sum_{n=0}^{\infty}\frac{(-1)^{s-1}}{s}\frac{1}{\lambda_n^s}s! = \sum_{n=0}^{\infty}\frac{(-1)^{s-1}}{\lambda_n^s}(s-1)!$$

$$\zeta_H(s) = \sum_{n=0}\frac{1}{\lambda_n^s} = \frac{(-1)^{s-1}}{(s-1)!}\frac{\partial^s}{\partial\lambda^s}\left(\log\left(\frac{\det(\hat{H}+\lambda)}{\det \hat{H}}\right)\right)\Big|_{\lambda=0}$$

- $$\frac{\det(\hat{H}_m+\lambda)}{\det(\hat{H}_m)} = \prod_{n=0}^{\infty}\left(1+\frac{\lambda}{\lambda_n}\right), \quad \lambda_n = \frac{(\mu_n^{(m)})^2}{R^2}$$

Положим $R=1$, тогда из 2 пункта:

$$\sum_{n=0}\frac{1}{(\mu_n^{(m)})^{2s}} = \frac{(-1)^{s-1}}{(s-1)!}\frac{\partial^s}{\partial\lambda^s}\left(\log\left(\frac{\det(\hat{H}_m+\lambda)}{\det \hat{H}_m}\right)\right)\Big|_{\lambda=0}$$

Повторяя рассуждения пункта 1, получим выражение (R=1):

$$\frac{\det(\hat{H}_m+\lambda)}{\det(\hat{H}_m)} = \frac{2^m m!}{\lambda^{\frac{m}{2}}}I_m(\sqrt{\lambda})$$

$$\sum_{n=0}\frac{1}{(\mu_n^{(m)})^{2s}} = \frac{(-1)^{s-1}}{(s-1)!}\frac{\partial^s}{\partial\lambda^s}\left(\log\left(\frac{2^m m!}{\lambda^{\frac{m}{2}}}I_m(\sqrt{\lambda})\right)\right)\Big|_{\lambda=0}$$

$$\sum_{n=0}^{\infty}\frac{1}{\left(\mu_n^{(0)}\right)^2} = \frac{\partial}{\partial\lambda}\left(\log\left(I_0(\sqrt{\lambda})\right)\right)\Big|_{\lambda=0} = \frac{\partial}{\partial\lambda}\left(\log\left(1+\frac{\lambda}{4}+...\right)\right)\Big|_{\lambda=0}$$

$$\sum_{n=0}^{\infty}\frac{1}{\left(\mu_n^{(0)}\right)^2} = \frac{1}{4}$$

$$\sum_{n=0}^{\infty}\frac{1}{\left(\mu_n^{(0)}\right)^4} = \frac{\partial^2}{\partial\lambda^2}\left(\log\left(I_0(\sqrt{\lambda})\right)\right)\Big|_{\lambda=0} = \frac{\partial^2}{\partial\lambda^2}\left(\log\left(1+\frac{\lambda}{4}+\frac{\lambda^2}{2^6}...\right)\right)\Big|_{\lambda=0}$$

$$\sum_{n=0}^{\infty}\frac{1}{\left(\mu_n^{(0)}\right)^4} = \frac{1}{32}$$

$$\sum_{n=0}^{\infty}\frac{1}{\left(\mu_n^{(1)}\right)^2}=\frac{\partial}{\partial\lambda}\left(\frac{2}{\sqrt{\lambda}}\log\left(I_1(\sqrt{\lambda})\right)\right)\Big|_{\lambda=0}=\frac{\partial}{\partial\lambda}\left(\log\left(\frac{2}{\sqrt{\lambda}}\left(\frac{\sqrt{\lambda}}{2}+\frac{\lambda^{\frac{3}{2}}}{2^4}+...\right)\right)\right)\Big|_{\lambda=0}$$

$$\sum_{n=0}^{\infty}\frac{1}{\left(\mu_n^{(1)}\right)^2}=\frac{1}{8}$$

20.2.4 Decay of a Metastable State (??)

(очень малонужная специфика)

ПТФ-19.у1 (30 б).

В этом упражнении мы будем работать с потенциалом, рассматриваемом на семинаре (????)
• **(10 б)** Вычислите соответствующее отношение функциональных определителей.
• **(20 б)** Найдите ширину уровней энергии для рассматриваемого на семинаре потенциале в квазиклассическом приближении. Сравните квазиклассическое приближение для основного состояния с найденным на семинаре ответом (см. комментарий к упражнению из семинара про двухъямный потенциал).

ПТФ-19.у2 (20 б).

Рассмотрите следующий интеграл, сходящийся при $\mathrm{Re}g>0$:

$$I(g)=\int\limits_{-\infty}^{\infty}dx\cdot\exp\left(-\frac{1}{2}x^2-gx^4\right)$$

• Постройте аналитическое продолжение этого интеграла на всю комплексную плоскость (включая область $\mathrm{Re}g<0$, где этот интеграл буквально расходится).
• Считая $g\ll 1$, найдите линии Стокса для построенного аналитического продолжения. Найдите асимптотическое поведение интеграла в различных секторах комплексной плоскости. Что можно сказать про вклады на самой линии Стокса?

ПТФ-19.з(50 б)

Рассмотрите распад метастабильного состояния частицы массы $m=1$ в потенциале $U(x)=\lambda x^2(\eta^2-x^2)$. Рассматривая Евклидову функцию Грина $G_E(0,0,\beta)$, найдите ширину уровня основного метастабильного состояния.
• **(20 б)** Найдите одноинстантонные траектории, соответствующую такому переходу, вычислите действия на них. Вычислите явно оператор, определяющий квадратичные флуктуации в окрестности инстантона.
• **(20 б)** Вычислите интегралы по нулевым модам, найдите соответствующий флуктуационный детерминант (используя метод Гельфанда-Яглома).
• **(10 б)** Просуммируйте разреженный инстантонный газ, найдите ответ.

20.3 Special Phenomena for Experiments

20.3.1 Problems about Blackbody Radiation and Photons

(Тут мощные задачи, которые нужно дня 4 продумывать. Это же в оптике будет. потом)

О3.2-1.1 Свойства черного тела

Рассматривая равновесное тепловое излучение как идеальный газ фотонов, содержащихся в вакуумированной полости с неподвижными непрозрачными стенками, имеющими постоянную температуру, получить формулу $P=\rho/3$, связывающую плотность энергии теплового излучения ρс давлением излучения P. Найти связь между энергетической светимостью R (интегральной излучательной способностью) абсолютно черного тела и плотностью энергии теплового излучения $\rho(T)$.

Solution

(в статфизе уже это выведено ведь? еще раз сделаю!)

О3.2-1.2 Свойства черного тела

Используя тот факт, что плотность энергии теплового излучения ρ не зависит от объема системы, а также формулу $P = \rho/3$, найти с помощью законов термодинамики зависимость ρ и энтропии s единицы объема от температуры T.

Solution

(???)

1.2* $\rho(T) = aT^4; s(T) = \frac{4a}{3}T^3$, где $a = \frac{4\sigma}{c}$.
Решение. Пусть равновесное тепловое излучение содержится в объеме V. Тогда его внутренняя энергия U и энтропия S соответственно равны

$$U(V,T) = \rho(T)V; S(V,T) = s(T)V$$

Воспользуемся термодинамическими тождествами

$$\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V; T\left(\frac{\partial S}{\partial T}\right)_V = C_V = \left(\frac{\partial U}{\partial T}\right)_V$$

Подставляя в первое из них уравнение состояния излучения $P = \rho(T)/3$ и соотношение (*), находим, что

$$s(T) = \frac{1}{3}\frac{d\rho}{dT}$$

Подставляя полученный результат и первое из соотношений (*) во второе тождество, находим уравнение для $\rho(T)$

$$\frac{d^2\rho}{dT^2} = \frac{3}{T}\frac{d\rho}{dT}$$

откуда $\rho(T) = aT^4$, а также

$$s(T) = \frac{1}{3}\frac{d\rho}{dT} = \frac{4}{3}aT^3$$

Полученная постоянная a в этих выражениях может быть выражена через постоянную Стефана - Больцмана $\sigma = 5,67 \cdot 10^{-5}$ эрг / $\left(\text{с} \cdot \text{см}^2 \cdot \text{К}^4\right)$. Интегральная плотность потока теплового излучения j [эрг/(см $^2 \cdot$ с)] зависит от температуры по закону Стефана-Больцмана $j = \sigma T^4$. Кроме того, $j = c\rho/4$ (см. задачу 1.1), откуда постоянная $a = 4\sigma/c = 7,56 \cdot 10^{-15}$ эрг/(см $^3 \cdot$ К^4).

Заметим, что соотношение $j = c\rho/4$ легко получить, если рассматривать излучение как идеальный газ фотонов, движущихся со скоростью c. Как известно из молекулярно-кинетической теории газов, плотность потока частиц, т. е. число частиц z, движущихся со средней тепловой скоростью $\bar{v}$ и пересекающих за 1 с единицу площади поверхности стенки сосуда, равно $z = n\bar{v}/4$. В этой формуле n - концентрация молекул газа, в нашем случае - это число фотонов в единице объема.

О3.2-1.3 Энтропия при расширении

Найти изменение энтропии равновесного теплового излучения абсолютно черного тела при расширении объема, занятого излучением, от V_1 до V_2 при постоянной температуре T.

Solution

(???)

1.3. $S_2 - S_1 = \frac{16\sigma}{3c}T^3(V_2 - V_1)$.

О3.2-1.4 Свойства черного тела

Используя формулы для энергии и энтропии равновесного теплового излучения, показать, что свободная энергия излучения может быть представлена в виде $\Psi = -AVT^4$, где V - объем, T - температура. Воспользовавшись законом Стефана-Больцмана, выразить A через постоянную Стефана-Больцмана σ. Пользуясь термодинамическими формулами, определить по найденному ч теплоемкость c_V фотонного газа в расчете на единицу объема и давление излучения P. Сравнить ее с теплоемкостью с $'$ единицы объема идеального одноатомного газа при одинаковых значениях P и T. Вычислить значение термодинамического потенциала Гиббса $\Phi = \Psi + PV$

Solution

(???)

1.4. $A = \frac{4\sigma}{3c}; c_V = \frac{16\sigma}{3c}T^3; P = \frac{4\sigma}{3c}T^4; c_V = 8c_V^{\text{ид.}}; \Phi = 0.$

О3.2-1.5 Цикл Карно фотонами (?????)

Найти работу, которую совершает в цикле Карно равновесное тепловое излучение абсолютно черного тела, полагая известными температуры «горячей» и «холодной изотерм T_1 и T_2, а также максимальный и минимальный объемы V_2 и V_1 системы на изотерме T_1.

Solution

(??по идее какая-то типичная термодинамика даст ответ, просто у нас другое ур. состояния?)

1.5. $A = \frac{16\sigma}{3c}T_1^3\,(T_1 - T_2)\,(V_2 - V_1).$

О3.2-1.6 Неон и фотоны

Газообразный неон находится в замкнутом сосуде постоянного объема в равновесии с тепловым излучением. При каком давлении P неона его теплоемкость равна теплоемкости теплового излучения в том же объеме при $T = 500$ К?

Solution

(???)

1.6. $P = \frac{32\sigma}{3c}T^4 = 1,26 \cdot 10^{-3}$ дин $/\text{см}^2 = 1,26 \cdot 10^{-4}\text{П} \approx 10^{-6}$ мм рт. ст.

О3.2-1.7 Теплоемкость и адиабата фотонов

Найти теплоемкость C_P и уравнение адиабаты фотонного газа, заключенного в сосуд с переменным объемом.

Solution

(???)

1.7. $C_P = \infty; VT^3 = \text{const}$ или $PV^{4/3} = \text{const}.$

О3.2-1.8 Температура фотонов

При какой температуре T давление равновесного теплового излучения равно $P = 1$ атм?

Solution

(? по идее где-то есть формула P(T).... такое нужно бы уметь делать??)

1.8. $T = \left(\frac{3c}{4\sigma}P\right)^{1/4} \approx 1,4 \cdot 10^5$ К.

О3.2-1.9 Концентрация газа для свойств фотона

При какой концентрации n молекул газа газокинетическое давление равно давлению равновесного теплового излучения при той же температуре $T = 300$ К?

Solution

(???)

1.9. $n = \frac{4\sigma}{3ck_\text{B}}T^3 \approx 1,8 \cdot 10^7\ \text{см}^{-3}.$

O3.2-1.10

При расчете теплоемкости C_V идеального газа, находящегося в равновесии с тепловым излучением в замкнутом сосуде постоянного объема, обычно пренебрегают вкладом равновесного излучения в теплоемкость системы. Найти отношение теплоемкостей C_y одноатомного газа и равновесного излучения, когда их давления одинаковы.

Solution

(???)

1.10. $\frac{C_V^{\text{ид}}}{C_V^{\text{идг}}} = \frac{1}{8}$.

O3.2-1.11 Сосуд, фотоны и поршень

Цилиндрический сосуд разделен на две части теплонепроницаемым поршнем, который может свободно перемещаться вдоль цилиндра герметично и без трения. В одной части сосуда находится идеальный газ, а в другой - равновесное тепловое излучение при температуре $T = 10^3$ K. Найти концентрацию атомов газа, если при малых изменениях температуры в обеих частях сосуда на одну и ту же величину направление смещения поршня не зависит or знака этой величины. Чему была равна начальная температура газа $T_{\text{г}}$?

Solution

(???)

Температуры в обеих частях сосуда разные. Запишем условие механического равновесия поршня

$$P_1 = nk_{\text{Б}}T_1 = \frac{4\sigma}{3c}T_2^4 = P_2$$

где индекс 1 относится к газу, а 2 - к излучению. Естественно предположить, что $T_1 \ll T_2$, так что давлением излучения при T_1 можно пренебречь. По условию задачи при малых изменениях температуры в обеих частях сосуда на одну и ту же величину направление смещения поршня не зависит от знака этой величины. Это означает, что в зависимости объема одной из частей сосуда от температуры имеется экстремум (минимум, если система устойчива), в окрестности которого $\partial V/\partial T = 0$. Так как $N = nV = \text{const}$, то в линейном приближении по отклонениям от равновесия $n\frac{\partial V}{\partial T} + V\frac{\partial n}{\partial T} = 0$, и, следовательно, $n/\partial T = 0$. Тогда из соотношения (*) следует

$$nk_{\text{Б}}\, dT_1 = \frac{16}{3c}\sigma T_2^3 dT_2$$

По условию задачи $dT_1 = dT_2$, откуда

$$n = \frac{16\sigma T_2^3}{3ck_{\text{Б}}} = 7,3 \cdot 10^{10}\ \text{см}^{-3}$$

Начальная температура газа $T_1 = T_2/4 = 250$ K. Поэтому отношение давлений излучения $\frac{P_1^{\text{изл}}}{P_2^{\text{изл}}} = \left(\frac{T_1}{T_2}\right)^4 = \frac{1}{256} \ll 1$, что оправдывает сделанное предположение о малости температуры газа в сравнении с температурой излучения.

ответ: 1.11* $n = \frac{16\sigma}{3ck_{\text{b}}}T^3 = 7,3 \cdot 10^{10}\ \text{см}^{-3}, T_{\text{г}} = \frac{T}{4} = 250$ K.

O3.2-1.12 Плоскость, шар и фотоны

Над плоскостью, зачерненной с обеих сторон, на высоте h расположен центр шара радиусом $a \propto h$, являющийся источником равновесного теплового излучения с температурой T_0. Найти стационарное распределение температуры на плоскости. Считать, что система находится в вакууме, фон теплового излучения отсутствует и теплопроводностью вдоль плоскости можно пренебречь.

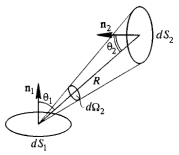
Solution

(???впишу в 1ю часть, не очевидный метод!! также в оптике это укажу!)

Поток энергии, излученный элементом поверхности dS_1, и падающий на элемент другой поверхности dS_2, определяется соотношением

$$d^2\Phi = \frac{B dS_1 ds_2 \cos\theta_1 \cos\theta_2}{R^2}$$

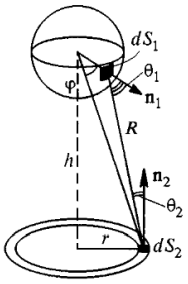
где в соответствии с рис. $200\mathbf{n}_1$ и $\mathbf{n}_2$ - единичные векторы нормалей к соответствующим площадкам, R - расстояние между площадками, B - коэффициент пропорциональности, называемый поверхностной яркостью (см. задачу 1.1), вообще говоря, зависящий от угла θ_1 (а также азимутального угла φ_1, не изображенного на рисунке).



угла φ_1, не изображенного на рисунке). Для абсолютно черного тела $B = \text{const}$ (закон Ламберта) и $B = \frac{\sigma T^4}{\pi}$. Если ввести телесный угол $d\Omega_2 = \frac{dS_2 \cos\theta_2}{R^2}$, под которым видна площадка dS_2 из центра первой плоIщадки, то

$$d^2\Phi = \frac{\sigma T^4}{\pi} dS_1 \cos\theta_1 d\Omega_2$$

На рис. 201 изображен шар - источник равновесного излучения, а под ним - зачерненная с обеих сторон поверхность, где и надо найти распределение температур.



Из соображений симметрии ясно, что $T = T(r)$. При условии $h \gg a$ телесный угол, под которым из центра шара видно кольцо радиусом r на плоскости

$$d\Omega_2 \simeq \frac{2\pi r dr \cos\theta_2}{R^2} = \frac{2\pi r dr}{h^2 r^2} \frac{h}{\sqrt{h^2 + r^2}}$$

Кроме того, условие $h \gg a$ позволяет считать, что $\theta_1 \approx \varphi$, где φ - угол между нормалью к dS_1 (т. е. радиусом) и вертикалью. Поэтому $dS_1 \cos\theta_1 \approx\approx dS_1 \cos\varphi = dS_1'$, где dS_1' - проекция dS_1 на экваториальную плоскость шара. Суммирование (интегрирование) по всем элементам полусферы дает πa^2. Поэтому поток излученной шаром энергии и поглощенный кольцом

$$d\Phi = \pi a^2 \frac{\sigma T_0^4}{\pi} \frac{2\pi r dr h}{\left(h^2 + r^2\right)^{3/2}}$$

В равновесии этот поток переизлучается кольцом по обе стороны плоскости:

$$d\Phi = 2\pi r dr \cdot 2\sigma T^4(r)$$

Из равенства этих потоков и следует ответ

$$T^4(r) = T_0^4 \frac{a^2 h}{2\left(h^2 + r^2\right)^{3/2}}$$

Ответ: 1.12* $T^4(r) = T_0^4 \frac{R^2 h}{2(h^2+r^2)^{3/2}}$.

О3.2-1.13

Решить предыдущую задачу, считая источником теплового излучения бесконечный круглый цилиндр радиусом a. Ось цилиндра параллельна плоскости и находится на расстоянии h от нее.

Solution

(???по идее для решения достаточно понять 1.12 задачу!)

O3.2-1.14

Над плоскостью, зачерненной с обеих сторон, на высоте h расположен круглый диск радиусом a, являющийся источником равновесного теплового излучения с температурой T_0. Радиус диска $a \propto h$, диск расположен параллельно плоскости. Найти стационарное распределение температуры $T = T(r)$ на плоскости, где r - расстояние от проекции центра диска. Считать, что система находится в вакууме, фон теплового излучения отсутствует и теплопроводностью вдоль плоскости можно пренебречь.

Solution

(???по идее для решения достаточно понять 1.12 задачу!)

O3.2-1.15

Имеются два полых тела, абсолютно отражающих снаружи и черных внутри. Оба тела имеют отверстия радиусом r и расположены на расстоянии $R (R \gg r)$. Первое тело имеет температуру T_1 и является единственным источником тепла для второго тела. Найти температуру второго тела T_2 при различных наклонах плоскостей отверстий по отношению k соединяющей их прямой. Насколько изменится T_2 при изменении угла наклона второго тела от 0 до 45*?

Solution

(???по идее для решения достаточно понять 1.12 задачу!)

O3.2-1.16

Два одинаковых абсолютно черных шарика расположены в вакууме на расстоянии $2l = 8$ см друг от друга. Посередине между двумя шариками помещена линза диаметром $D = 6$ cm, собирающая излучение одного шарика на поверхность другого. Один из шариков раскален до температуры $T_1 = 2000$ K. Определить температуру другого шарика, пренебрегая фоном теплового излучения и потерями в линзе.

Solution

(???по идее для решения достаточно понять 1.12 задачу!)

O3.2-1.17

В сферической оболочке диаметром D имеется отверстие диаметром $d \propto D$. Внутренняя поверхность оболочки рассеивает излучение диффузно по закону Ламберта с коэффициентом рассеяния $\rho < 1$. Определить коэффициент поглощения A, характеризующий отверстие для внешнего наблюдателя. При каком отношении диаметров d/D коэффициент поглощения A будет отличаться от I меньше, чем на $0,1\%$, если $\rho \approx 1$?

Solution

(???по идее для решения достаточно понять 1.12 задачу!)

O3.2-1.18 Нагревание линзой (!?!?!??!)

Линза со светосилой 1:16 (это отношение D^2/F^2) собирает солнечный свет на поверхность черного шарика, помещенного в вакуум. До какой температуры T может нагреться шарик, диаметр которого равен диаметру изображения Солнца? Считать Солнце абсолютно черным телом с температурой $T_\mathrm{C} = 6000$ K.

Solution

(???)

Вычислим величину телесного угла Ω, под которым была бы видна линза из центра Солнца. Пусть L - расстояние от Солнца до Земли, а D - диаметр линзы. Угол α, под которым из центра Солнца виден радиус линзы, равен $\alpha = D/2L$, отсюда

$$\Omega = 2\pi(1 - \cos\alpha) = 4\pi \sin^2 \frac{\alpha}{2} \approx \pi\alpha^2 = \pi \left(\frac{D}{2I}\right)^2$$

Плотность потока энергии, излучаемой с поверхности Солнца, $j = \sigma T_{\text{C}}^4$. Поток энергии, излучаемой с поверхности Солнца в единицу телесного угла, равен $\frac{\sigma T_{\text{C}}^4 4\pi R_{\text{C}}^2}{4\pi}$. Мощность солнечного излучения, падающего на линзу,

$$N_{\text{C}} = \sigma T_{\text{C}}^4 R_{\text{C}}^2 \pi \left(\frac{D}{2L}\right)^2$$

Нагреваясь, шарик, излучает. Когда поток энергии, полученной от Солнца, сравняется с потоком излученной энергии, установится равновесная температура шарика. Поток энергии с поверхности шарика диаметром d

$$N_{\text{Ш}} = \sigma T^4 4\pi \frac{d^2}{4}$$

По условию размер изображения Солнца $\alpha_C F$ равен диаметру d шарика, где $\alpha_C = \frac{2R_C^2}{L}$ - угловой размер Солнца, а F - фокусное расстояние линзы. Таким образом,

$$N_{\text{m}} = \sigma T^4 \pi d^2 = \sigma T^4 \pi \alpha_{\text{C}}^2 F^2 = \sigma T^4 \pi F^2 \frac{4R_{\text{C}}^2}{L^2}$$

Приравнивая потоки энергии N_{C} и $N_{\text{ш}}$, получаем

$$\sigma T_{\text{C}}^4 R_{\text{C}}^2 \pi \frac{D^2}{4L^2} = \sigma T^4 F^2 \pi \frac{4R_{\text{C}}^2}{L^2}$$

откуда и находим искомую температуру шарика

$$T = \frac{T_{\text{C}}}{2}\sqrt{\frac{D}{F}} = 1500 \text{ K}$$

Ответ: 1.18* $T = \frac{T_{\text{C}}}{2}\sqrt{\frac{D}{F}} = 1500$ K.

О3.2-1.19 Нагревание воздушного шара

Объектив диаметром $D = 5$см и фокусным расстоянием $F = 5$ см фокусирует солнечный свет на абсолютно черный шар диаметром $d = 1$ мм, обладающий высокой теплопроводностью и находящийся в высоком вакууме вне Земли, на ее орбите. Определить температуру T шара. Принять, что плотность потока солнечной энергии равна $J_{\text{C}} = 0,14\text{Вт/см}^2$, температура стенок сосуда $T_0 = 300$ K. Потерями энергии в объективе пренебречь. Угловой размер Солнца $a_{\text{C}} = 0,01$ рад.

Solution

(???)

1.19. $T = T_0 \left(1 + \frac{j_{\text{C}} D^2}{4\sigma T_0^4 d^2}\right)^{1/4} \approx 1980$ K.

О3.2-1.20

Найти отношение плотностей потоков энергии корпускулярного и электромагнитного излучения Солнца в околоземном пространстве. Считать, что корпускулярный поток представляет собой нейтральную плазму из протонов и электронов с концентрацией $n = 5\ \text{см}^{-3}$ частиц каждого сорта и скоростью потока $v = 300$ км/с, а Солнце - источник равновесного теплового излучения с температурой $T = 6000$ K. Выразить результат через угловой размер α_{C} Солнца, т. е. угол, под которым с Земли виден диаметр Солнца ($\alpha_{\text{C}} = 0,01$ рад).

О3.2-1.21

Солнечная постоянная $J_{\text{С}}$ означает мощность излучения, падающего на единицу площади, помещенной перпендикулярно солнечным лучам за пределами земной атмосферы на расстоянии от Солнца, равном среднему расстоянию межау Землей и Солнцем $L = 1,5 \cdot 10^8$ км. Принимая $J_{\text{С}} = 0,14\text{ВТ}/\text{ см }^2$ и радиус Солнца $R_{\text{С}} = 7 \cdot 10^5$, определить радиационную температуру $T_{\text{раа}}$ излучающей поверхности Солнца.

О3.2-1.22

Спектр излучения космического рентгеновского источника соответствует спектру излучения абсолютно черного тела. Максимум плотности излучения $\rho(\lambda)$ наблюдается на длине волны $\lambda_{\max} = 2$ А, а суммарная по спектру (интегральная) плотность потока на Земле $j = 10^{-11}\text{В}/\text{см}^2$. Расстояние от Земли до источника $L = 1,3 \cdot 10^4$ световых лет. Оценить диаметр источника.

О3.2-1.23

Абсолютно черное тело подвешено в вакуумной установке так, что через оптическое окно на него падает солнечный свет. Если стенки установки охладить до температуры $T_{\text{ст}} = 77$ К, то тело будет иметь $T_1 = 275$ К. Найти температуру тела T_2 при $T_{\text{ст}2} = 295$ К. Теплопроводностью остаточных газов и подвески пренебречь.

О3.2-1.24

На графитовый шарик радиусом $r = 1$ см, подвешенный точно в центре сферы с зеркальными стенками, находящейся в околоземном пространстве, с помощью линзы фокусируется изображение Солнца (рис. 66). Радиус сферы $R = 0,25$М, диаметр линзы $D = 2,5$ cm, фокусное расстояние линзы $F = 0,25$, угловой размер Солнца $\alpha_{\text{С}} = 10^{-2}$, температура поверхности Солнца $T_{\text{С}} = 6 \cdot 10^3$ К. Считая графит абсолютно чер- ным телом, найти установившуюся темпера- туру шарика T

О3.2-1.25

. Хорошо теплопроводящий шар с за- черненной поверхностью находится в косми- ческом пространстве на некотором расстоянии r от центра Солнца. Найти температуру шара, если он находится or Солнца на расстояниях, равных радиусам орбит Венеры, Земли, Марса и Юпитера, равных (в млн км) $R_{\text{В}} = 108, R_3 = 150, R_{\text{М}} = 228$, $R_l = 780$. Солнце считать источником равновесного теплового излучить полученные величины с радиоастрономическими данными: средЗемли, Марса и Юпитера оцениваются, соответственно, как $T_{\text{В}} = 735$ К, $T_3 = 275$ К, $T_{\text{М}} = 235$ К и $T = 135$ К. Чем можно объяснить большое расхождение рассчитанной таким образом и полученной в измерениях температуры поверхности Венеры?

О3.2-1.26

Оценить температуру Солнца, исходя из его видимого углового размера $a_{\text{С}} = 0,01$ рад и температуры земной поверхности ($T_3 \simeq 300$ К)

О3.2-1.27

Космонавт оказался в свободном пространстве в тени Земли. Считая что его организм в процессе нормальной жизнедеятельности выделяет мощность $W = 100$ВТ, оценить скорость изменения температуры космонавта. Коэффициент отражения скафандра $\varepsilon = 0,95$.

О3.2-1.28

Межпланетная станция имеет оболочку в форме шара диаметром $2r = 1$ м. На борту станции находится радиопередатчик моцностью $N = 200$Вт с КПД $\eta = 50\%$. Станция заполнена теплообменным газом. Аппаратура станции может работать в интервале температур $t = -50 \div 100°$С. Определить, при каких удалениях L от Солнца станция может работать: 1) при кратковременных включениях; 2) в непрерывном режиме. Какова должна быть отражательная способность а поверхности станции, чтобы станция могла работать при сколь угодно большом удалении от Солнца? Радиус Солнца $R_{\text{С}} = 7 \cdot 10^5$; считать, что оно излучает как абсолютно черное тело с температурой $T_{\text{С}} = 6000$ К.

О3.2-1.29

В свободном пространстве находится железная пластина, одна поверхность которой абсолютно «чернаяэ, а другая - идеально

О3.2-1.42

Слой вещества поглощает практически все фотоны солнечного спектра с энергией $\mathscr{E} \geqslant 0,2$ эВ и полностью прозрачен для фотонов с меньшей энергией. Оценить, какую долю x солнечной энергии пропускает вещество. Считать спектр Солнца планковским с температурой $T = 6000$ К.

О3.2-1.43

Слой вещества поглощает практически все фотоны солнечного спектра с энергией § $\geqslant$ 12 эВ и полностью прозрачен для фотонов с меньшей энергией. Оценить, какую долю x солнечной энергии пропускает вещество. Считать спектр Солнца планковским с температурой $T = 6000$ К.

О3.2-1.44

Поверхность некоторого тела приготовлена таким образом, что коэффициент поглощения электромагнитного излучения $A = 1$ для частот $\omega \leqslant \omega_0$ и $A = 0$ при $\omega > \omega_0$. Это тело помещено в вакуум и в отсутствии аругих источников излучения нагревается за счет внутреннего источника энергии до температуры T. Определить эту температуру, если известно, что для такого же тела с абсолютно черной поверхностью в тех же условиях равновесная температура $T^* = 300$ К. Граничная частота соответствует температуре $\theta = \hbar\omega_0/k_5 = 300$ К.

О3.2-1.45

Частотная зависимость коэффициента поглощения A некоторого тела, имеющего внутренний источник энергии, изображена на рис. 70. Это тело помещено в космическом пространстве вдали от источников излучения. Такое же тело, но с абсолютно черной поверхностью, нагревается там до температуры $T^* = 100$ К. Определить температуру тела, если величины ω_1 и ω_2 соответствуют энергиям квантов 0,015 эВ и 0,6 эВ. дется в направлении, перпендикулльрном илоскости слоя. Піри какой толщине d слоя Рис. 70 ся равной 90% интенсивности равновесного излучения? Линейный коэффициент поглощения данной длины волны $x = 0,1$ cm^{-1}. Показатели преломления плазмы и окружающей среды считать при этом одинаковыми.

О3.2-1.47

Излучение Солнца регистрируется селективным приемником на длине волны $\lambda = 300$ нм с относительной шириной области чувствительности $\Delta\lambda/\lambda = 10^{-3}$ за промежутки времени $\tau = 10^{-3}$с. Найти относительную среднеквадратичную флуктуацию принимаемого сигнала. Солнце считать абсолютно черным телом с температурой $T = 6000$ К и видимым угловым размером $\alpha_C = 0,01$. Площадь, приемной площадки равна $S = 1$ мм^2. [2].

Указание. Так как энергия кванта $\hbar\omega \gg k_5 T$, то среднее планковское число заполнения (среднее число фотонов) $\bar{n}_\infty$ &1, и поэтому к фотонам можно применять классическую, а не квантовую статистику.

О3.2-1.48

Радиоизлучение из межзвездного пространства (реликтовое излучение) регистрируется приемником с фиксированной относительной полосой пропускания $\Delta v/v = \text{const}$. Оказалось, что при переходе от приема на длине волны $\lambda_1 = 3$ cm приему на длине волны $\lambda_2 = 0,3$ см величина сигнала возросла в 400 раз, причем при дальнейшем небольшом уменьшении λ увеличилась незначительно. Исходя из этих данных, определить температуру реликтового излучения, считая его равновесным тепловым излучением. Во сколько раз изменится сигнал при переходе от $\lambda = 3$см$\lambda = 30$ cm?

Указание. Корнем уравнения $e^x - 2,5x = 1$, которое возникает при решении задачи, является $x \approx 1,62$.

О3.2-1.49

Лазер на рубине излучает в импульсе длительностью $\tau = 0,5$ мс энергию $= 10$ Дж в виде почти параллельного светового пучка сечением $S = 1$ cm^2. Рабочая длина волны лазера $\lambda = 6943$Å, ширина линии $\Delta\lambda = 0,01$ Å. Определить по спектральной плотности пучке а) до фокусировки, б) при максимально возможном сужении пучка (в фокусе).

О3.2-1.50

Определить температуру абсолютно черного тела, спектральная яркость излучения которого равна яркости лазерного излучения с энергией в импульсе $\mathscr{E} = 1$ Дж. Считать, что расходимость лазерного пучка определяется только дифракцией на выходном отверстии, а немонохроматичность - длительностью импульса.

O3.2-1.51

При какой температуре интенсивность излучения поверхности абсолютно черного тела в соответствующем спектральном интервале (энергия, уносимая с единицы поверхности в единицу времени в единицу телесного угла) сравнится с интенсивностью лазера с плотностью потока энергии $j = 1$ мВт/см ^{2} и относительной стабильностью частоты $\Delta v/v = 10^{-12}$, работающего на длине волны $\lambda = 6900$ А? Диаметр пучка принять равным $d = 1$ cm.

O3.2-1.52

Оценить эффективную температуру гелий-неонового лазера, генерирующего в непрерывном режиме свет с шириной спектраль ной линии $\partial v = 10^4$ Гц. Мощность излучения лазера $W = 1$ мВт.

O3.2-1.53

Измерение интенсивности реликтового излучения Вселенной производится радиоскопом вблизи $\lambda = 3$ см. Его антенный тракт находится при температуре $T = 300$ K и поглощает $a = 1\%$ поступающей мощности. Какой аффективной температуре абсолютно черного тела T_{eff} соответствует тепловой шум антенного тракта в области данной длины волны?

Solution

(???)

O3.2-1.54

Атом Na находится в пучке лазерного света с плотностью потока энергии j и длиной волны $\lambda = 0,59$ мкм, совпадающей с одной из спектральных линий Na. Время спонтанного испускания Na для этой линии $\tau = 16$ нс. При больших плотностях потока $j > j_0$ ускорение a, приобретаемое атомом за счет давления света, перестает зависеть от j. Оценить значение плотности потока насыщения j_0. Определить также предельную величину a. Доплеровским сдвигом частоты при излучении движущегося атома пренебречь.

Solution

(???)

O3.2-1.55

. Возбужденный атом с энергией возбуждения & = 1 эВ находится в поле равновесного излучения с температурой $T = 300$ K. Найти отношение вероятностей индуцированного и спонтанного излучений атома. Найти аналогичное отношение для электронного спина в магнитном поле с индукцией $B = 10^3$Гс.

O3.2-1.56 Когда спонтанное вероятнее индуцированного

Определить диапазон частот излучения, при котором вероятность спонтанного перехода более чем в 100 раз превосходит вероятность индуцированного перехода под влиянием равновесного излучения температуры $T = 293$ K.

Solution

(???)

O3.2-1.57

Система, состоящая из атомов, имеющих два невырожденных уровня энергии $\oint_1$ и $\oint_2 > \oint_1$, находится в тепловом равновесии. Выразить коэффициент поглощения света $\varkappa(T, \omega)$ этой системой на частоте $\omega = (_2 - _1)/h$ через его значение x_0 при $T = 0$. Рассмотреть два предельных случая: 1) $k_{\text{b}}T \gg h\omega$ и 2) $k_{\text{b}}T \& h\omega$.

Solution

(???)

O3.2-1.58

Оценить вероятность $W_{\text{сп}}$ спонтанного излучения молекулы при переходе с возбужденного уровня $\oint_n$ на уровень $\oint_m$ в случае, когда молекула помещена внутрь объемного резонатора, настроенного на частоту $\omega = (\delta_n - \delta_m)/h$. Соответствующая вероятность спонтанного излучения в свободном пространстве равна $W^0_{\text{сп}}$ Объем резонатора равен V, его добротность - Q. Считать, что ширина Γ молекулярных уровней все время остается меньше ширины ω/Q линии резонатора: $\Gamma < \omega/Q$. Сделать численную оценку для случаев: 1) $V = 1$ см$^3, \lambda = 1$ см, $Q = 10^4$ и 2) $V = 1$ см$^3, \lambda = 1$ мкм, $Q = 10^6$.

Solution

(???)

O3.2-1.59

Резонатор лазера с кристаллом рубина имеет одно зеркало со 100%-ным отражением, а другое - с коэффициентом пропускания $\tau = 0,1$ на длине волны, отвечающей генерации лазера. Длина кристалла $l = 12$ см. Известно, что коэффициент поглощения света в невозбужденном кристалле рубина в максимуме рабочей линии равен $k_n = 0,4$ см$^{-1}$. Найти, какую часть атомов хрома нужно перевести в возбужденное состояние, чтобы лазер начал работать. Рассеянием света в кристалле пренебречь.

Solution

(???)

O3.2-1.60 Перестройка частоты

В спектре энергетических уровней молекулы воды есть два уровня A и B с разностью энергий δ_{0+} между которыми разрешены оптические переходы. Создавая в разреженном водяном паре при температуре $T = 300$ К тлеющий разряд, не нагревающий пар, можно получить инверсную заселенность этих уровней. На этом основана работа лазера, в котором электромагнитная волна с частотой $v_0 = \delta_0/h = 8,48 \cdot 10^{11}\Gamma$ усиливается по мощности на длине резонатора в $\beta_0 = 1,04$ раз. Расстояние между зеркалами резонатора можно слегка менять, регулируя тем самым собственную частоту резонатора. Коэффициент отражения каждого из зеркал $R = 0,99$. Определить возможную перестройку частоты излучения лазера, принимая во внимание эффект Доплера, обусловленный тепловым движением молекул.

Solution

(???)

O3.2-1.70

. Зеркальный металлический прямоугольный волновод с поперечным сечением 34×72 мм и длиной $L =$ 10 м замкнут накоротко с обоих концов и через малое отверстие соединен с абсолютно черной полостью, нагретой до температуры $T = 600$ К. Оценить плотность электромагнитной Энергии в волноводе (в эрг/Гц) в диа пазоне длин волн 10 см.

O3.2-1.71. Время жизни черной дыры (??)

Как показал в 1974 г. С. Хокинг, черная дыра массой M за счет квантовых эффектов и конечных размеров излучает как абсолютно черное тело с температурой $T(M) = hc^3/(8\pi k_{\text{ь}}\psi M)$. Оценить время жизни черной дыры с массой $M = 10^{15}$г до ее полного испарения.

Solution (????)

O3.2-1.72

Яркая желто-зеленая линия полярного сияния (aurora borealis) возникает при возбуждении атомов кислорода в верхних слоях атмосферы под действием солнечного ветра (потока быстрых электронов и протонов). Время жизни возбужаенного состояния атома кислорода относительно спонтанного перехода составляет т $\simeq 0,74$с. Однако столкновения атомов кислорода с молекулами атмосферы могут снять это возбуждение безызлучательным способом. Эффективное сечение этого процесса $\sigma \simeq 7 \cdot 10^{-15}$ см^2. Оценить, на какой высоте над Землей «загорается эта линия. Атмосферу считать изотермической с $T = 240$ К

O3.2-1.73

Рекомбинация ионов и злектронов в межзвездной среде приводит к образованию атомов в высоковозбужденных состояниях с главным Квантовым числом $n > 1$ (ридберговских атомов). При переходах с $\Delta n = 1$ очень высоковозбужденные атомы излучают радиоволны, что было обнаружено в 1964 г радиотелескопом РТ-22 в г. Пущино.

В межзвездной среде есть и изотропное магнитотормозное излучение со спектральной интенсивностью в коротковолновом радиодиапазоне $I(\omega) \simeq 2{\cdot}10^{-15} \frac{\text{эрт}}{\text{с}^2\ \text{см}^2\text{с}^{-1}}$. Оценить максимально возможное n для атома водорода в этих условиях. Спонтанное время жизни высоковозбужденных состояний атома водорода в вакууме (с $n \sim 10^3$) равно $\tau_{cu}(n) \simeq 6 \cdot 10^{-12} n^5$с.

O3.2-1.74

Взаимодействие электрона в атоме водорода с нулевыми колебаниями электромагнитного поля в вакууме, приводящее в частности к расщеплению по энергии состояний $2s_{1/2}$ и $2p_{1/2}$ (лэмбовский сдвиг) можно в интервале частот $\left(Ry/\hbar, 2mc^2/\hbar\right)$ рассматривать, кақ взаимодействие свободного электрона с однородным переменным электромагнитным полем, которое приводит к случайным смещениям электрона на орбите. Оценить величину среднеквадратичного смещения электрона.

20.3.2 Problems about line widths and their detection 1

O3.1-5.1 Естественная ширина

Среднее время жизни атома в возбужденном состоянии составляет около $\tau \sim 10^{-8}$ с. При переходе атома в основное состояние испускается фотон, средняя длина волны которого равна $\lambda = 500$ нм. Оценить ширину $\Delta\lambda$ и относительную ширину $\Delta\lambda/\lambda$ излучаемой спектральной линии, если не происходит ее уширения за счет других процессов.

5.

1. $\Delta\lambda \sim \frac{\lambda^2}{c\Delta t} \sim 10^{-4}$НМ, $\quad \frac{\Delta\lambda}{\lambda} \sim \frac{\lambda}{c\Delta t} \sim 10^{-7}$.

O3.1-5.2 Излучение π-мезоатома

В π-мезоатоме водорода роль электрона играет отрицательный пион π^-, энергия покоя которого составляет 140 МэВ. Оценить связанную с распадом пиона относительную ширину спектральной линии, соответствующей переходу пиона с L на K-оболочку. Время жизни пиона равно $2,6 \cdot 10^{-8}$с.

5.

2. $\frac{\Delta\lambda}{\lambda} \approx \frac{\hbar}{\tau E_{21}} \approx 1,4 \cdot 10^{-11}$, где $E_{21} = \frac{3}{8}\mu c^2\alpha^2; \mu = \frac{m_\pi m_\text{p}}{m_\pi + m_\text{p}}; \alpha$ - постоянная тонкой структуры.

O3.1-5.3 Размер решетки для естественную ширины

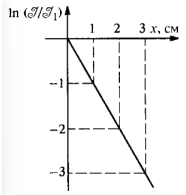
Оценить минимальную ширину L_min, которую должна иметь дифракционная решетка, чтобы с ее помощью можно было обнаружить естественную ширину линии, испускаемой атомами с временем жизни возбужденного состояния $\tau = 0,1$ нс. (Все условия постановки опыта предполагаются идеальными.)

5.

3. $L_{\min} = c\tau = 3$ cm.

О3.1-5.4

Моноэнергетический параллельный пучок возбужденных атомов движется вдоль оси вакуумной трубки со скоростью $v = 10^8$см/с. В стенках трубки сделаны окошки для регистрации излучения атомов пучка в зависимости от пути, пройденного атомами. Результаты этих измерений изображены на рис. ниже



По оси абсцисс отложено расстояние x, пройденное атомами вдоль трубки, отсчитанное от 1-го окошка, а по оси ординат - натуральный логарифм отношения интенсивности света $\mathcal{J}$ интенсивности $\mathcal{J}_1$, измеренной детектором, стоящим в 1-м окошке. Определить естественную ширину линии Δv, излучаемой атомами пучка.

5.

4. $\Delta v \approx \tau^{-1} = 10$ МГц, где $\tau = -\frac{\Delta x}{v\Delta(\ln \mathscr{G}/\mathscr{O})}$.

О3.1-5.5 Температура водородного облака

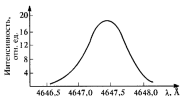
Температуру газовых облаков в межзвездном пространстве можно оценить по доплеровскому уширению спектральных линий, испускаемых атомами, входящими в состав газа. Для этой цели обычно используют водородную линию с длиной волны $\lambda = 21$ см (см. также тексты задач 6.48 и 6.50, объясняющие природу этой линии). Оценить температуру T газового водородного облака, если испускаемая им водородная линия имеет полуширину $\Delta v = 5$ кГц.

5.

5. $T \approx \frac{m_{\text{p}}\lambda^2(\Delta v)^2}{4k} \approx 33$ К.

О3.1-5.6.

На рис. 37 изображено распределение энергии в спектральной линии дважды ионизованного углерода ^{12}с (эту спектральную линию можно наблюдать в дуговом разряде в сильном магнитном поле). Уширение спектральной линии обусловлено движением излучающих атомов (эффект Доплера). Оценить температуру T излучающих атомов.



5.

6. $T = \left(\frac{\Delta\lambda}{\lambda}\right)^2 \frac{\mu c^2}{4R} = 8 \cdot 10^5$ К, где R - универсальная газовая постоянная, $\Delta\lambda$ - ширина на половине высоты резонансной кривой.

О3.1-5.7

Изучается спектр излучения газа в разрядной трубке. Считая, что при столкновениях возбужденные атомы мгновенно переходят в нижележащие состояния, оценить соотношение между доплеровской шириной спектральных линий в диапазоне видимого света и их уширением за счет столкновений, если длина свободного пробега $l \approx 10^{-4}$см.

5.

7. $\frac{\Delta\lambda_\mu}{\Delta\lambda_{\text{ст}}} = \frac{2l}{\lambda} \approx 3,6.$

О3.1-5.8

Возбужденные атомы с временем жизни $\tau \sim 10^{-10}$с и энергией ионизации $\mathscr{E}_{\text{и}} \sim 10$ эВ ионизуются излучением с длиной волны $\lambda \sim 100$Å. Оценить относительный разброс фотоэлектронов по энергиям.

5.

8. $\frac{\delta\mathscr{E}}{\hbar\omega - \mathscr{E}_{\text{ион}}} \approx \frac{\hbar/\tau}{2\pi\hbar c/\lambda - \mathscr{E}_{\text{ион}}} \approx 6 \cdot 10^{-8}.$

О3.1-5.9 Уширение от столкновений

Одна из причин уширения спектральных линий атомов в газе связана со столкновениями, которые ограничивают время жизни возбужденного состояния. Оценить вклад этого механизма в относительную ширину линии перехода в неоне на длине волны $\lambda = 0,63$ мкм, используемой в гелий-неоновом газовом лазере, в условиях, когда коэффициент диффузии атомов неона $D = 100\text{см}^2/\text{с}$. Температуру газа принять равной $T = 400$ К.

5.

9. $\frac{\Delta\nu}{\nu} = \frac{kT\lambda}{m_{\text{Ne}}Dc} \approx 3,5 \cdot 10^{-8}.$

О3.1-5.10

Молекула CO_2 имеет множество дискретных переходов, пригодных для генерации лазерного излучения вблизи 1000см^{-1} с расстоянием между линиями $\Delta q \approx 2\text{см}^{-1}$. Для осуществления плавной перестройки частоты лазера пользуются повышенным давлением, когда ударное уширение приводит к слиянию этих линий в одну полосу. Оценить необходимое для этого давление P при температуре $T = 400$ К Сечение столкновения молекул $\sigma \approx 10^{-15}\text{см}^2$.

5.

10* $P \approx \frac{2\pi c\Delta q}{\sigma}\sqrt{\frac{MkT}{3}} \approx 440$ атм.

Решение. Ударное уширение спектральных линий связано с тем, что при определенных давлениях газа время жизни атомов в возбужденном состоянии определяется временем между столкновениями молекул

$$\tau \sim \frac{l}{v_{\text{T}}} \approx \frac{1}{n\sigma v_{\text{T}}}$$

где l - длина свободного пробега молекул, $v_{\boldsymbol{\tau}}$ - среднеквадратичная скорость молекул, соответствующая температуре T, т. е. $v_\tau = \sqrt{3kT/M}, n$ - концентрация, σ - сечение столкновений. Таким образом, необходимое давление

$$P = nkT \approx \frac{kT}{\sigma v_{\text{T}}\tau} = \frac{1}{\sigma\tau}\sqrt{\frac{MkT}{3}}$$

С другой стороны, время жизни атомов в возбужденном состоянии, определяемое столкновениями атомов, и уширение спектральных линий связаны соотношением неопределенностей: $\Delta\boldsymbol{v}_{\text{ст}}\,\tau \approx 1$ (или $\Delta\omega_{\text{ст}}\,\tau \approx 2\pi$).

Если расстояние между спектральными линиями (в обратных сантиметрах) Δq станет равным ударному уширению, то произойдет слияние этих линий, т. е.

$$\Delta v_{\text{ст}} \gtrsim \Delta v = \Delta\left(\frac{c}{\lambda}\right) = 2\pi c \Delta q, \quad \text{где} \quad q = \frac{2\pi}{\lambda} \gg \Delta q.$$

Отсюда искомое время жизни $\tau^{-1} \approx 2\pi c \Delta q$. Окончательно необходимое для слияния линий давление

$$P = \frac{1}{\sigma\tau}\sqrt{\frac{MkT}{3}} \approx \frac{2\pi c \Delta q}{\sigma}\sqrt{\frac{MkT}{3}} \approx 440 \cdot 10^6 \text{ дин } /\text{см}^2 \approx 440\text{а}.$$

О3.1-5.11

В опытах с разными молекулами измерялись энергии перехода между тремя последовательными уровнями энергии вращательной полосы двухатомной молекулы (рис. 38a и б). Найти квантовые числа I этих уровней и момент инерции I молекулы в случаях а и б.

5.

11. а) $l = 0, 1, 2; I = 6,9 \cdot 10^{-39}\Gamma \cdot \text{ см}^2$.
б) $l = 1, 2, 3; I = 13,8 \cdot 10^{-39}\Gamma \cdot \text{ см}^2$.

О3.1-5.12

Из опыта известно отношение длин волн электромагнитного излучения, соответствующего переходам в молекулах HCl и HI из основного в первое вращательное востояние: $\alpha = \lambda_{\text{HCl}}/\lambda_{\text{HI}}$ Определить отношение междуядерных расстояний в этих молекуsax $x = r_{\text{HCl}}/r_{\text{HI}}$.

5.

12. $x = \sqrt{\alpha \frac{\mu_{\text{HJ}}}{\mu_{\text{HCl}}}} \approx 1,01\sqrt{\alpha}$, где μ - приведенная масса молекулы.

О3.1-5.13

Какова максимальная длина волны СВЧ-излучения, с помощью которой можно вызвать переход между ротационными уровнями молекул хлора? Расстояние между ядрами атомов в молекуле Cl_2 равно $a = 2 \cdot 10^{-8}$см. Относительная атомная масса изотопа хлора $A = 35$.

О3.1-5.14

Найти отношение частот линий поглощения наиболее длинноволновых вращательных переходов молекулы HCl для двух изотопов хлора ^{35}Cl и ^{37}Cl. Считать, что межатомные расстояния не зависят от изотопического состава молекулы. Вычисления произвести с точностью $10^{-2\%}$

О3.1-5.15

Найти отношение наименьших энергий переходов между вращательными уровнями газа, состоящего из смеси водорода и дейтерия, в котором присутствуют молекулы H_2, HD и D_2. Считать, что межатомное расстояние не зависит от изотопического состава.

О3.1-5.16 Переходы между вращательными

Дальний инфракрасный спектр молекулы HBr, обусловленный переходами между соседними вращательными уровнями молекул, состоит из ряда линий, отстоящих друг от друга на расстояние $\Delta\left(\frac{1}{\lambda}\right) = 17\text{см}^{-1}$. Найти расстояние между ядрами в моле куле HBr.

О3.1-5.17

Оценить в видимой области спектра ($\lambda = 6000$Å) разрешающую способность R спектрального прибора, пригодного для исследования спектра молекулярного водорода (т. е. спектра, обусловленного переходами между электронновращательными уровнями молекулы). Момент инерции молекулы H_2 в основном электронном состоянии $I = 0,46 \cdot 10^{-40}\text{г} \cdot \text{см}^2$.

О3.1-5.18

При каких величинах периода вращения T песчинки с характерным размером $a = 0,1$ мкм начинает проявляться квантовый характер вращения, т. е. дискретность вращательного спектра? Плотность песчинки ρ принять равной $5/\text{cm}^3$.

О3.1-5.19

При температурах ниже приблизительно $T = 100$ K молярная теплоемкость C_V молекулярного водорода составляет $3R/2$, тогда как при комнатных температурах она равна $5R/2$(R - универсальная газовая постоянная). Пользуясь этими данными, оценить момент инерции I молекулы водорода относительно оси, проходящей через ее центр перпендикулярно к оси, проходящей через атомы, из которых построена молекула. Оценить также частоты v и длины волн λ спектральных линий, возникающих при переходах между вращательнымн уровнями молекулы.

О3.1-5.20

Оценить количество вращательных уровней молекулы HCl, возбуждаемых при комнатной температуре. Межъядерное расстояние у этой молекулы равно $d = 1,27$Å.

О3.1-5.21

Показать, что в основном состоянии гармонического осциллятора $\overline{\Delta p^2} \cdot \overline{\Delta x^2} = \hbar^2/4$, где $\overline{\Delta p^2}$ и $\overline{\Delta x^2}$ - среднеквадратичные отклонения импульса и координаты от их средних значений. Волновая функция основного состояния гармонического осциллятора $\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \exp\left(-\frac{\alpha x^2}{2}\right)$, где $\alpha = \frac{m\omega}{\hbar}$ Смотрите также задачу 2.43.

О3.1-5.22

Показать, что уравнение Шредингера, описывающее одномерный гармонический осциллятор, помещенный в однородное электрическое поле $\mathbf{E}$, может быть сведено к задаче о гармоническом осцилляторе, т. е. движению в потенциале вида $U = m\omega^2 x^2/2$. Каковы уровни энергии частицы в этом случае?

О3.1-5.23

В спектре испускания молекулярного азота имеются линии с длинами волн 3371 Å, 3577 Å и 3805Å. Можно ли интерпретировать Эти линии как переходы с изменением колебательного квантового числа на 0,1 и 2, если измерения сделаны с точностью $0,2\%$? Определить энергетическое расстояние между соответствующими уровнями молекулы азота. С помощью полученных результатов по формулам классической физики оценить жесткость k упругой связи атомов в молекуле азота.

О3.1-5.24

Оценить отношение кванта колебаний молекул H_2 и O_2 к характерной энергии возбуждения валентных электронов $\mathscr{E}_e$, считая, что эффективный коэффициент упругости молекулярной связи $k = \mathscr{E}_\text{e}/a^2$, где a - межатомное расстояние. Выразить ответ через отношение массы электрона m к массе ядра M. Оценить амплитуду нулевых колебаний молекул и выразить ее через отношение m/M и a.

О3.1-5.25 Параметры газа CO по пику поглощения на данной длине волны

В угарном газе CO из-за возбуждения колебаний молекул наблюдается пик поглощения инфракрасного излучения на длине волны $\lambda = 4,61$ мкм. Определить амплитуду A_0 нулевых колебаний молекулы CO. Оценить температуру, при которой амплитуда тепловых колебаний превзойдет A_0.

Теорема вириала тут используется.

О3.1-5.26

Какова амплитуда колебаний молекулы кислорода O_2 при комнатной температуре, если известно, что расстояние между ее колебательными уровнями равно $\Delta\mathscr{E} = 0,25$ эВ?

О3.1-5.27

На рис. 39 изображена часть графика зависимости энергии взаимодействия U атомов азота друг с другом от межатомного расстояния r. Считая яму параболической, найти отношение колебательного кванта к энергии возбуждения первого вращательного состояния в молекуле азота.

О3.1-5.28

Пылинка с плотностью $\rho = 2$ г/см ^{3} и радиусом r прикреплена к неподвижной стенке невесомым стержнем длиной $l = 4r$ и диаметром $d = 2r = 1$ мкм (рис. 40). Модуль Юнга стержня $E = 10^{11}$ Па. Определить энергию кванта колебаний пылинки вдоль нормали к стенке, а также длину электромагнитной волны, способной возбудить такие колебания, и амплитуду нулевых колебаний.

О3.1-5.29

Разность энергий диссоциации молекул D_2 и H_2 равна $\Delta\mathscr{E} = 0,08$ эВ, а потенциал взаимодействия атомов в этих молекулах одинаков. Каковы энергии нулевых колебаний этих молекул (в эВ)?

О3.1-5.30

Оценить энергию нулевых колебаний атомов жидкого гелия (плотность $\rho = 0,145$ г/см ^{3}).

О3.1-5.31

Определить отношение энергий возбуждения первого вращательного уровня молекулы азота в основном и первом возбужденном колебательном состояниях. Расстояние между атомами азота в основном состоянии молекулы $r_0 = 1,1$Å, квант вибрационных возбуждений $\hbar\omega = 0,3$ эВ.

О3.1-5.32

Поле, в котором движется атом жидкого гелия, хорошо описывается потенциалом Леннард-Джонса $U(r) = \varphi\left[(r_0/r)^{12} - -2\,(r_0/r)^6\right.$, где $\varphi = 232$ К, а $r_0 = 3 \cdot 10^{-8}$ см. Оценить энергию нулевых колебаний.

О3.1-5.33 Колебания атоме, описываемым потенциалом Морса (??)

Потенциал взаимодействия атомов в двухатомной молекуле можно с достаточной точностью аппроксимировать потенциалом Морса $U(r) = D\left[\exp\left(-2\alpha\left(r - r_0\right)\right) - 2\exp\left(-\alpha\left(r - r_0\right)\right)\right]$. У молекулы азота постоянная $\alpha = 4 \cdot 10^8 \text{см}^{-1}$, энергия диссоциации равна $D = 7,4$ эВ. Оценить расстояние между колебательными уровнями молекулы азота.

О3.1-5.34

Смесь атомов двух видов A и B имеет уровни возбужденных с частотой v, такой что $hv = \mathscr{E}_A$, кроме последующего обратного излучения той же частоты в результате соударений атомов A и B появ- 45 ляется также излучение с частотой $v' = \mathscr{E}_B/h$ и происходит увеличение кинетической энергии атомов. Найти скорости атомов после соударений, если известны массы атомов m_A и m_B. Считать, что энергия теплового движения мала по сравнению с $\Delta\wp$.

О3.1-5.35

При лазерном разделении изотопов в газообразной фазе один из разделяемых изотопов ионизуется лазерным лучом и затем удаляется из смеси электростатическим полем. Такому разделению изотопов препятствует тепловое движение атомов. Определить, возможно ли подобное разделение изотопов ^{6}Li и ^{7}Lic помощью ультрафиолетового лазера, если известно, что энергия ионизации лития 5,4 эВ; газообразный литий может существовать при температуре $t^\circ \geqslant 800°$c. Принять, что Z_{eff} для электрона незаполненной оболочки не зависит от массы изотопа.

О3.1-5.36

В атоме тантала ($Z = 73$) совершается переход с M-слоя на L-слой. Определить длину волны λ испущенного фотона, если постоянная экранирования $\sigma = 5,5$.

О3.1-5.37

Вычислить приближенно частоту и длину волны K_α-линии Mo, а также энергию кванта, соответствующую этой линии.

О3.1-5.38

Найти приближенно минимальное напряжение V на рентгеновской трубке, при котором начинают появляться K_α-линии Mo, Cu, Fe.

O3.1-5.39

Найти границу K-полосы излучения Mo, Cu и Fe.

O3.1-5.40

Какие линии Ni возбуждаются K-излучением Co?

O3.1-5.41

Известно, что длина K_α-линии одного элемента равна 0,0788 нм, а другого 0,0713 нм. Выяснить, стоят ли эти элементы рядом в таблице Менделеева. Какие Это элементы?

O3.1-5.42

Начиная с какого элемента появляется L-серия?

O3.1-5.43

Определить напряжение V на рентгеновской трубке с никелевым антикатодом, если разность длин волн между K_α-линией и коротковолновой границей сплошного рентгеновского спектра равна $\Delta\lambda =$ 84НМ.

20.3.3 Problems about line widths and their detection 2

O3.1-5.44

Какой минимальной кинетической энергией должна обладать α-частица, чтобы при бомбардировке такими частицами атомов лития ^{7}Li эти атомы начали излучать полный спектр своего характеристического рентгеновского излучения?

5.

44. $T_{\min} = \frac{m_e c^2 \alpha^2 (Z-1)^2}{2[1-m_\alpha/(m_{\mathrm{Li}}+m_\alpha)]} = 85,5$ эВ, где α - постоянная тонкой структуры.

O3.1-5.45

Какова максимальная скорость v электронов, вырываемых из свинца характеристическим излучением железа?

5.

45. $v \approx 5 \cdot 10^9$ cm/c.

O3.1-5.46

У каких элементов характеристическое рентгеновское излучение длинноволновой границы K-серии может испытывать брэгговское отражение от кристалла LiF, постоянная решетки которого $d = 0,23$ нм?

5.

46. Минимальное значение Z находится из условия Брэгга-Вульфа $\lambda \leqslant 2d \quad (m = 1)$. Тогда $Z_{\min} = 18$.

O3.1-5.47

Какой потенциал V следует приложить к рентгеновской трубке, чтобы тормозное рентгеновское излучение могло испытывать брэгговское отражение от кристалла LiF, межплоскостное расстояние в котором составляет $d = 2,3$Å?

5.

47. $V \geqslant \frac{hc}{2ed}; V_{\min} = 2,7\text{кВ}$.

О3.1-5.48

Длина волны, соответствующая переходу между двумя соседними состояниями вращательного спектра молекулы HBr, равна $\lambda = 202$ мкм. Определить, между состояниями с какими квантовыми вращательными числами происходит переход. Межъядерное рассто- яние $d = 1,41$Å.

5.

48. Переход из $l = 3$ в $l = 2$.

О3.1-5.49

Оценить, при какой температуре отношение числа молекул NO, находящихся в чисто вращательных состояниях с квантовыми числами $l = 1$ и $l = 0$, равно $\alpha = 0,1$. Межъядерное расстояние в молекуле равно $d = 1,15$Å.

О3.1-5.50

С какой относительной точностью $\Delta\lambda/\lambda$ надо измерить длинноволновую часть вращательного спектра CO, чтобы увидеть изотопическое расщепление спектра, появляющееся при наличии примеси ^{12}c^{17}O в обычном ^{12}c^{16}O? Чему равна наибольшая длина волны вращательного кванта у молекул CO? Расстояние между ядрами с и O равно $d = 1,13$Å

О3.1-5.51

Природный хлор представляет собой смесь двух изотопов ^{35}Cl и ^{37}Cl. С какой относительной точностью $\Delta\lambda/\lambda$ надо измерять длину волны колебательного кванта у молекулы HCl, чтобы увидеть изотопическое расщепление колебательного спектра?

О3.1-5.52

Одномерный осциллятор находится в состоянии с главным квантовым числом $n = 10$. Оценить, какова вероятность обнаружить частицу вблизи положения равновесия в области размером порядка плюс-минус амплитуда его нулевых колебаний.

Ука з а и ие. При больших квантовых числах движение частицы можно рассматривать как классическое.

О3.1-5.53

Одномерный осциллятор находится в основном состоянии. Оценить вероятность нахождения частицы в классически разрешенной области. Волновая функция основного состояния $\psi = A\exp\left(-x^2/2a_0^2\right)$, где $a_0 = \sqrt{\hbar/m\omega}$.

Ука за н и е. Для оценки получающегося интеграла использовать разложение подынтегральной функции в ряд.

О3.1-5.54

Для молекулы азота N_2 оценить число вращательных уровней, приходящихся на интервал между соседними колебатель ными уровнями.

О3.1-5.55

Потенциальная энергия взаимодействия атомов в двухатомной молекуле не является чисто квадратичной (гармонической). При слабой ангармоничности уровни осциллятора можно представить в виде $_n = \hbar\omega(n + 1/2) - \alpha\hbar\omega(n + 1/2)^2$, где α - коэффициент ангармоничности, ω - частота осциллятора. Найти в Этой модели максимальное число колебательных уровней молекулы N_2, у которой $\alpha = 0,006145$.

Указан и е. Для реальных состояний функция $\mathscr{E}_n(n)$ должна быть монотонно возрастающей.

О3.1-5.56

Из-за конечного размера ядра энергетический уровень K электрона претерпевает небольшое смещение $\delta\mathscr{E} \propto R^2$, где R - рааиус ядра, который находится по формуле $R = 1,3 \cdot 10^{-13} A^{1/3}$см, A - относительная атомная масса. Оценить величину изотопического сдвига $\delta(hv)_{205}$ границы характеристического рентгеновского K-из.уучения для ядра $^{205}_{805}$Tl, если известно, что для $^{203}_{81}$Tl этот сдвиг 47 $\delta(hv)_{203} = -8,25$ эВ, т. к. энергия ионизации K-электрона уменьшается по сравнению со случаем точечного ядра.

О3.1-5.57

Считая, что взаимодействие атомов в молекуле HCl описывается потенциалом Кратцера $U(r) = 2\varepsilon\left[\frac{1}{2}\left(\frac{\sigma}{r}\right)^2 - \frac{\sigma}{r}\right]$, определить относительное изменение частоты $\frac{\Delta\omega}{\omega_0}$ колебаний молекулы при возбуждении ее с вращательного уровня c$l = 0$ на уровень $l = 10$. В молекуле HCl$\varepsilon = 4,62$ эВ $, \sigma = 1,27$Å.

О3.1-? Разрешающая способность прибора для различения колебательного спектра

Природный бром представляет собой смесь двух изотопов ^{79}Br(50.56%) и ^{81}Br(49.44%).

Оценить разрешающую способность спектрального прибора, с помощью которого можно различить изотопическое расщепление колебательного спектра поглощения паров брома.

Бром это двухатомная молекула, каждая из которой может быть своим изотопом.

колебательная энергия есть

$$E_{\text{кол}} = \hbar\omega(n + 1/2)$$

При этом частота зависит от приведенной массы как $\omega = \sqrt{\frac{k}{\mu}}$, так что нулевой уровень колебательной энергии разный для разных молекул. Также и частота перехода зависит от молекулы, соответственно её спектр тоже.

k одинаковая, потому что оно определяется электромагнитным взаимодействием и электронами, так что оно одинаково для разных изотопов.

разрешающая способность есть (вообще говоря модуль от)

$$R = \frac{\lambda}{\Delta\lambda} = \frac{\omega}{\omega_2 - \omega_1}$$

находим

$$\Delta\omega = \sqrt{k}\left(\frac{1}{\sqrt{\mu_1}} - \frac{1}{\sqrt{\mu_2}}\right)$$

$$R = \frac{1}{\frac{\omega_2}{\omega_1} - 1} = \frac{1}{\sqrt{\frac{\mu_1}{\mu_2}} - 1}$$

и считаем разные приведенные массы.

в итоге $R = 160$.

(потом в оптике качну про разрешающие способности)

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5.

13. $\lambda_{\max} = \frac{\pi c A m_{\text{p}} a^2}{\hbar} \approx 2,1$ cm.

5.

14. $\frac{\omega_{35}}{\omega_{37}} = \frac{I_{37}}{I_{35}} = 1,0015$, где индексы 35 и 37 относятся к изотопам хлора ^{35}Cl и ^{37}Cl, I - моменты инерции молекул относительно центра масс.

5.

15. $\mathscr{E}_{\text{H}_2} : \mathscr{E}_{\text{HD}} : \mathscr{E}_{\text{D}_2} = 2 : \frac{3}{2} : 1$.

5.

16. $r = \left(\frac{\hbar}{2\pi\mu_{\mathrm{HBr}}c\Delta}\right)^{1/2} = 1,4 \cdot 10^{-8}$c, где $\mu_{\mathbf{HBr}} \approx m_{\mathrm{p}}$ - приведенная масса молекулы HBr .

5.

17. $R = \frac{\lambda}{\Delta\lambda} = \frac{\omega}{\Delta\omega} = \frac{2\pi cI}{\hbar\lambda} \approx 140$, т. е. требуемая разрешающая способность $R > 140$. Такое разрешение может быть получено в спектрометре, использующем призму.

5.

18. $T \geqq \frac{\rho a^5}{\hbar} \approx 500$c.

5.

19. Решение. Теплоемкость молекулярного водорода $\mathbf{C} = C_{\text{пост}} + C_{\text{вр}} + C_{\text{кол}}$. Поскольку расстояния между колебательными уровнями велики ($\Delta\mathscr{E}_{\text{кол}} \sim \sqrt{\frac{M}{m}}\Delta\varrho_{\text{вр}} \approx 40\Delta\mathscr{E}_{\text{вр}}$), то при комнатных температурах колебательные уровни не возбуждены, а вращательные уровни возбуждены все, поскольку по условию $C_V = (5/2)R$. При $T = 100$ K вращательные уровни не возбуждены вовсе. Таким образом,

$$kT \lesssim \Delta\mathscr{E}_{\text{Вр}} = \frac{\hbar^2}{I}, \quad \text{откуда} \quad I \leqq \frac{\hbar^2}{kT} \sim 10^{-40}\Gamma \cdot \text{ cm}^2$$

где k - постоянная Больцмана. Следовательно,

$$h\nu = \frac{\hbar^2}{2l}2(l+1) \approx kT(l+1); \quad \nu = \frac{kT}{h}(l+1), \quad \text{где} \quad l = 0, 1, 2, ...;$$

$$\nu_{\min} \approx \frac{kT}{h} \approx 2,1 \cdot 10^{12}\Gamma, \quad \lambda_{\max} \approx 1,5 \cdot 10^{-2} \text{ cm} = 0,15\text{m}$$

Соответствующая линия лежит в далекой инфракрасной области спектра.

5.

20. Количество вращательных уровней $l_{\max} \simeq 4$.

5.

22: $\mathscr{E}_n = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{e^2E^2}{2m\omega^2}$, где $n = 0, 1, 2, ...$

Решение. Запишем уравнение Шредингера для одномерного гармонического осциллятора в электрическом поле $\mathbf{E}$

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \left(\frac{m\omega^2x^2}{2} - eEx\right)\psi.$$

Перепишем его в таком виде:

$$\widehat{H}\psi = -\frac{\hbar^2}{2m}\psi'' + \frac{m\omega^2}{2}\left(x^2 - \frac{2eE}{m\omega^2}x\right)\psi.$$

Полученное уравнение можно свести к уравнению колебаний осциллятора со смещенным положением равновесия, если выделить полный квадрат в выражении в скобках в правой части уравнения

$$x^2 - \frac{2eE}{m\omega^2}x = \left(x - \frac{eE}{m\omega^2}\right)^2 - \frac{E^2e^2}{m^2\omega^4} = (x^*)^2 - \frac{e^2E^2}{m^2\omega^4}.$$

Тогда уравнение Шредингера примет вид

$$-\frac{\hbar^2}{2m}\psi'' + \frac{m\omega^2}{2}\left(x - \frac{eE}{m\omega^2}\right)^2 \psi = \left(\hat{H} + \frac{e^2E^2}{2m\omega^2}\right)\psi$$

или

$$-\frac{\hbar^2}{2m}\psi'' + \frac{m\omega^2}{2}x^{*^2}\psi = \mathfrak{E}^*\Psi.$$

Уровни энергии в этом случае, очевидно, следующие:

$$\mathscr{E}_n^* = \hbar\omega\left(n + \frac{1}{2}\right), \quad \text{или} \quad \mathscr{E}_n = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{e^2E^2}{2m\omega^2}, \quad \text{где} \quad n = 0, 1, 2, ...$$

5.

23: $\omega_1 - \omega_2 = \omega_2 - \omega_3 = \Omega = 0,32 \cdot 10^{15}\mathrm{c}^{-1} = \sqrt{k/\mu}$, откуда вычисляем $k \approx 1,2 \cdot 10^6$ дин/см.
Решение. Найдем частоты, соответствующие заданным переходам (рис. 156),

$$\omega_1 = \frac{2\pi c}{\lambda_1} = 5,59 \cdot 10^{15}\mathrm{c}^{-1}$$
$$\omega_2 = \frac{2\pi c}{\lambda_2} = 5,27 \cdot 10^{15}\mathrm{c}^{-1}$$
$$\omega_3 = \frac{2\pi c}{\lambda_3} = 4,95 \cdot 10^{15}\mathrm{c}^{-1}$$

При вычислении мы сделаем округление в третьем знаке. Это дает точ ность $(0,01/5) \cdot 100\% = 0,2\%$, что укладывается в интервал измерений ($0,2\%$ - по условию). Вычислим разности частот

$$\omega_1 - \omega_2 = 0,32 \cdot 10^{15}c^{-1}; \quad \omega_2 - \omega_3 = 0,32 \cdot 10^{15}c^{-1}$$

Такое совпадение указывает на эквидистантность уровней $1, 2, 3$. Следовательно, они могут быть связаны с колебательными уровнями молекулы

$$\omega_1 - \omega_2 = \omega_2 - \omega_3 = \Omega = \sqrt{\frac{k}{\mu}}$$

где k - жесткость упругой связи, μ - приведенная масса молекулы N_2. Таким образом, искомая жесткость

$$k = \mu\Omega^2 = 1,2 \cdot 10^6 \text{ дин } /, \text{ где } \mu = 11,69 \cdot 10^{-24}.$$

Заметим, что найденный колебательный квант молекулы азота Вращат $\Delta\mathscr{E} = \hbar\Omega = 0,21$ эВ. Табличное значение 0,29 эВ.

5.

24: $\frac{\hbar\omega_0}{\mathrm{e}} \approx 2\sqrt{\frac{2m_\mathrm{e}}{M}}$; $A \approx a\sqrt[4]{\frac{m_\mathrm{e}}{M}}$, где M - масса атома.
Решение. Двухатомную молекулу можно рассматривать как квантовый гармонический осциллятор. На рис. 157 изображен потенциал взаимодействия атомов в такой молекуле. Вблизи положения равновесия форма ямы приближенно параболическая. Однако из-за соотношения неопределенностей квантово-механическая система не может находиться в этом положении - на дне потенциальной ямы. В результате возникают нулевые колебания с полной энергией $\mathscr{E}_0 = \hbar\omega_0/2$. Далее идут эквидистантные

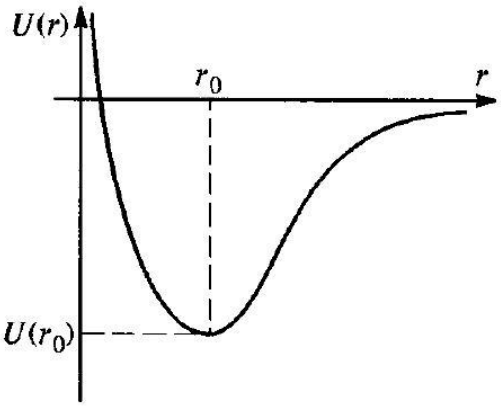


Рис. 157 уровни возбужденных состояний двухатомной молекулы с $\Delta\mathscr{E} = \hbar\omega_0$, где ω_0 частота колебаний двухатомной молекулы $\omega_0 = \sqrt{k/\mu} = \sqrt{2k/M}$, где k - коэффициент упругой молекулярной связи, μ приведенная масса молекулы, M - масса атома в молекуле типа H_2 или O_2.

Согласно соотношению неопределенностей и теореме вириала для осцилятора можно записать $\mathscr{E}_e \sim 2\frac{p^2}{2m_e} \sim \frac{\hbar^2}{m_e a^2}$ (считаем, что область локализации электрона порядка межатомного расстояния). Отсюда искомое отношение

$$\frac{\hbar\omega}{\mathscr{E}_e} = \frac{\hbar\sqrt{2k/M}}{\mathscr{E}_e} = \sqrt{2\frac{\hbar^2}{a^2 m_e M \mathscr{E}_e}\frac{m_e}{M}} \sim \sqrt{\frac{2m_e}{M}} \approx \begin{cases} 0,035 \text{ для } H_2 \\ 0,01 \text{ для } O_2 \end{cases}$$

Для оценки амплитуды нулевых колебаний воспользуемся приведенной в условии соотношением $k = \mathscr{E}_e/a^2$. Как указывалось выше, энергия нулевых колебаний

$$\mathscr{E}_0 = \frac{\hbar\omega_0}{2} = \frac{kA^2}{2}, \quad \text{откуда} \quad A^2 = \frac{\hbar\omega_0 a^2}{\mathscr{E}_e}$$

Подстановкой найдем

$$A \approx a\sqrt[4]{\frac{m_e}{M}} \approx \begin{cases} 0,15a \text{ для } H_2 \\ 0,08a \text{ для } O_2 \end{cases}$$

Величина $K = \sqrt[4]{\frac{m_e}{M}}$ носит название параметра неадиабатичности (см. задачу 5.29).

5.

25. $A_0 = \sqrt{\frac{\hbar\lambda}{2\pi c\mu}} \approx 4,74 \cdot 10^{-10}$c; $T \geqq 3100$ K.

5.

26. Молекула O_2 находится в основном состоянии, так как $kT = 0,025$ В $\ll \Delta\mathscr{E}$. Поэтому $A_0 = \frac{\hbar}{\sqrt{\mu\Delta\mathscr{E}}} = 0,058$Å, где μ - приведенная масса O_2.

5.

27. $\frac{\Delta\mathscr{E}_{\text{кол}}}{\Delta\mathscr{E}_{\text{вр}}} = \frac{\mu r_0^2\omega}{\hbar} \approx 180$, где μ - приведенная масса молекулы азота, r_0 - положение минимума кривой, берется из графика.

5.

28. $\lambda = 2\pi c\sqrt{\frac{4lr\rho}{3\varrho}} \approx 31$ cm; $\hbar\omega = 4 \cdot 10^{-6} \ni$ В; $A_0 = \sqrt{\frac{\hbar}{m\omega}} = \sqrt{\frac{\hbar}{\pi r^2}\sqrt{\frac{3}{\mathscr{G}\rho}}} \approx \approx 4 \cdot 10^{-13}$ cm.

5.

29: $\mathscr{E}_{\text{OH}} = \frac{\hbar\omega_{\text{H}}}{2} = \frac{\sqrt{2}\Delta\mathscr{E}}{\sqrt{2}-1} = 0,27_{\text{эВ}}; \mathscr{E}_{\text{OD}} = \frac{\hbar\omega_{\text{D}}}{2} = \frac{\Delta\mathscr{E}}{\sqrt{2}-1} = 0,19$ эВ.

Решение. Поскольку масса электрона много меньше массы ядер, то скорости движения последних малы по сравнению со скоростями электронов. Тогда в первом приближении можно найти энергию электронов при неподвижных ядрах, а затем учесть движение ядер. Такой подход носит название адиабатического приближения.

Энергия молекулы с учетом движения ядер может быть записана как $\mathscr{E} = \mathscr{E}_{\text{эл}}(R) + \mathscr{E}_{\text{яд}}^{\text{кии}} + \mathscr{E}$. При этом энергия электронов зависит от межъядерного расстояния как от параметра. В энергию $\mathscr{E}(R)$ включена также энергия электростатического отталкивания ядер, поэтому $\mathscr{E}_{\text{эл}}(R)$ фактически является полной энергией молекулы при фиксированном положении ядер. Полагая далее, что $R = R_0 + \delta R$, где R_0 - равновесное расстояние между ядрами, а δR - отклонение от него вследствие движения ядер, запишем $\mathscr{E}_{\text{эл}}(R) \approx \approx \mathscr{E}(R_0) + \frac{1}{2}\frac{\partial^2\mathscr{E}(R)}{\partial R^2}\Big|_{R=R_0}(\delta R)^2$. Второй член представляет собой потенциальную энергию ядер $U_{\text{яд}}^{\text{пот}}$, т. е. усредненный потенциал, создаваемый электронами. Вместе с кинетической энергией они образуют энергию колебаний $\mathscr{E}_{\text{яд}}^{\text{кин}} + U_{\text{яд}}^{\text{пот}} = \mathscr{E}_{\text{кол}}$. Если сюда добавить энергию вращения молекулы как целого $\mathscr{E}$, то получим энергию молекулы в адиабатическом приближении $\mathscr{E} = \mathscr{E}(R_0) + \mathscr{E}_{\text{кол}} + \mathscr{E}_{\text{вр}}$. Заменяя по принципу соответствия классические выражения двух последних членов их квантовыми аналогами, получим

$$\mathscr{E}_0 = \mathscr{E}_{9\Omega}(R_0) + \hbar\omega_{\text{кол}}\left(n + \frac{1}{2}\right) + Bl(l+1)$$

где $B = \frac{\hbar^2}{2\mu R_0^2}$ - постоянная вращения, μ - приведенная масса ядер, $\omega_{\text{кол}}^2 = \frac{1}{\mu}\frac{\partial^2\mathscr{E}(R)}{\partial R^2}\Big|_{R=R_0}$ - квадрат частоты колебаний ядер. Можно показать, что $\mathscr{E}_{\text{эл}}(R_0) : \hbar\omega_{\text{кол}} : B = 1 : K^2 : K^4$ (см. задачу 5.24).

Энергия диссоциации - это разница между энергиями основного состояния молекулы и энергии двух удаленных атомов водорода (дейтерия), принимаемую равной нулю. Т.о. $I = \mathscr{E}_0$. Энергия основного состояния молекулы $\mathscr{E}_0 = \mathscr{E}(R_0) + \frac{1}{2}\hbar\omega_{\text{кол}}$. Разность энергий диссоциаций молекул D_2 и H_2

$$\Delta\mathscr{E} = I_{\text{D}_2} - I_{\text{H}_2} = 2\mathscr{E}_{\text{D}} - 2\mathscr{E}_{\text{эл. D}}(R_0) - \frac{\hbar\omega_{\text{D}}}{2} - 2\mathscr{E}_{\text{H}} + 2\mathscr{E}_{\text{эл. H}}(R_0) + \frac{\hbar\omega_{\text{H}}}{2}.$$

Поскольку

$$\mathscr{E}_{\text{D}} - \mathscr{E}_{\text{H}} = \frac{e^4}{2\hbar^2}(\mu_{\text{D}} - \mu_{\text{H}})$$

где $\mu = \frac{m_{\text{e}}M}{m_{\text{e}}+M} \approx m_{\text{e}}\left(1 - \frac{m_{\text{e}}}{M}\right)$ - приведенная масса электрона, то с учетом одинаковости потенциалов взаимодействия, получим

$$\Delta\mathscr{E} \approx \hbar\frac{\omega_{\text{H}} - \omega_{\text{D}}}{2} = \frac{\hbar\omega_{\text{D}}}{2}\left(\frac{\omega_{\text{H}}}{\omega_{\text{D}}} - 1\right).$$

Отношение $\frac{\omega_{\text{H}}}{\omega_{\text{D}}} = \sqrt{\frac{\mu_{\text{D}}}{\mu_{\text{H}}}} = \sqrt{2}$, откуда следует $\frac{\hbar\omega_{\text{D}}}{2} = \frac{\Delta\mathscr{E}}{\sqrt{2}-1} \approx 0,19$ эВ и $\frac{\hbar\omega_{\text{H}}}{2} = \sqrt{2}\frac{\Delta\mathscr{E}}{\sqrt{2}-1} = 0,27^{\text{g}}$В.

5.

30. $_0 \approx \frac{3\hbar^2}{8mr^2} \approx 1,2\cdot10^{-16}$ эрг $= 0,75\cdot10^{-4}{}_{\text{эВ, где } 2r} \approx 4,5\cdot10^{-8}$ см характерный размер области, занимаемый одним атомом в жидком гелии, $2r \approx \left(\frac{6\mu}{\pi\rho N_{\text{A}}}\right)^{1/3}$.

5.

31*: $\frac{\Delta\mathscr{E}_{\text{вр}}}{\Delta\mathscr{E}_{\text{кол}}} = \frac{\hbar}{\omega\mu r_0^2} = 1,63\cdot10^{-3}$.

Решение. С ростом номера колебательного возбуждения меняется средний квадрат расстояния между атомами в молекуле и, следовательно, момент инерции молекулы (рис. 158) зависит от n.

$\mathscr{E}_{\text{кол}} = \hbar\left(n + \frac{1}{2}\right) = \langle K\rangle + \langle U\rangle = 2\langle U\rangle$ - теорема вириала. Далее, $\langle U\rangle = 2\frac{\mu\omega^2}{2}\langle x_n^2\rangle \to \langle x_n^2\rangle = \frac{\hbar}{\mu\omega}\left(n + \frac{1}{2}\right)$, где

μ - приве-

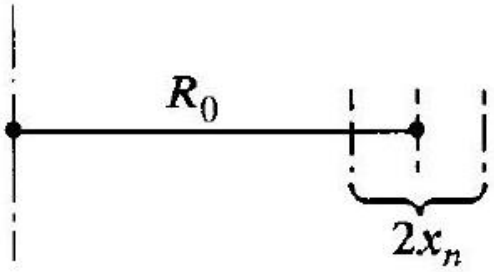


Рис. 158 денная масса ядер. При этом $\left\langle x_0^2 \right\rangle = \frac{1}{2}\frac{\hbar}{\mu\omega} = \frac{A_0^2}{2}$ (см. задачу 5.25). Тогда

$$\sqrt{\langle x_0^2 \rangle} = \sqrt{\frac{1}{2}\frac{\hbar^2}{\mu\hbar\omega}} = 10^{-9}\ \text{cm} = 0,1\text{Å} \ll 1,1\text{Å} = r_0.$$

Среднее значение вращательной энергии

$$\left\langle \frac{1}{2I} \right\rangle \hbar^2 l(l+1) = \frac{\hbar^2}{2\mu} l(l+1) \left\langle \frac{1}{r_n^2} \right\rangle \approx \frac{\hbar^2}{2\mu} \frac{l(l+1)}{\langle r_n^2 \rangle}.$$

Надо отметить, что усреднение ведетсяя по заданному колебательному состоянию. В силу адиабатичности, $\mathscr{E}_{\text{вр}}$ - поправка к $\mathscr{E}_{\text{кол}}$.

Последнее равенство $\left(\left\langle \frac{1}{r_n^2} \right\rangle \approx \frac{1}{\langle r_n^2 \rangle}\right)$ справедливо, поскольку для небольших $n < 100$ справедливо соотношение $\left\langle x_n^2 \right\rangle \ll r_0$.

$$\Delta\mathscr{E}_{\text{Вр}}(l=1, \to l=0) = \frac{\hbar^2}{\mu \left\langle r_n^2 \right\rangle}$$

$$\frac{\Delta\varrho_{\text{Вр}}(n=0)}{\Delta\mathscr{G}_{\text{Вр}}(n=1)} = \frac{\left\langle (r_0 + x_1)^2 \right\rangle}{\left\langle (r_0 + x_0)^2 \right\rangle} = \frac{\left\langle r_0^2 + 2x_1 r_0 + x_1^2 \right\rangle}{\left\langle r_0^2 + 2x_0 r_0 + x_0^2 \right\rangle} = \frac{r_0^2 + \left\langle x_1^2 \right\rangle}{r_0^2 + \left\langle x_0^2 \right\rangle} =$$

$$= \frac{r_0^2 + 3\hbar/(2\mu\omega)}{r_0^2 + \hbar/(2\mu\omega)} \approx \left(1 + \frac{3}{2}\frac{\hbar}{\mu\omega r_0^2} - 1 - \frac{1}{2}\frac{\hbar}{\mu\omega r_0^2}\right) = \frac{\hbar}{\mu\omega r_0^2} = 1,63 \cdot 10^{-3}$$

Как видно из решения, существует взаимодействие между вращением и колебаниями ядер, что соответствует выходу за пределы адиабатического приближения (см. задачи 5.29 и 5.57).

5.

32. $\mathscr{E}_0 = \frac{3\hbar\omega}{2} = 3\hbar\sqrt{\frac{18\varphi}{mr_0^2}} = 1,944 \cdot 10^{-2} \ni$ В ≈ 226 К.

5.

33. $\Delta\mathscr{E}_{\text{кол}} = \hbar\alpha\sqrt{\frac{4D}{m}} \approx 0,3$ эВ.

5.

34. $v_{\text{A}} = \sqrt{\frac{2\Delta\varrho m_{\text{B}}}{m_{\text{A}}(m_{\text{A}}+m_{\text{B}})}}$; $\quad v_{\text{B}} = \sqrt{\frac{2\Delta\varrho m_{\text{A}}}{m_{\text{B}}(m_{\text{A}}+m_{\text{B}})}}$, где $\Delta\mathscr{E} = h\,(v - v')$.

5.

35. Разность энергий ионизации атомов $^6_3$Li и $^7_3$Li$\Delta\mathscr{E} = 7 \cdot 10^{-5}$ эВ; ширина линии поглощения из-за эффекта Доплера $2\hbar\Delta\omega \approx \hbar\omega\frac{v}{c} \approx \approx 4,4 \cdot 10^{-5}$, точнее (с учетом коэффициента $2\sqrt{\ln 2}$, см. Д. В. Сивухин «Общий курс физики. Оптика», формула 89.11) 5,1710-5 эВ. Поскольку $\Delta\mathscr{E} > \hbar\Delta\omega$ (при $t \approx 800°$C), разделение изотопов возможно.

5.

36. $\lambda = \frac{hc}{\mathrm{Ry}(Z-\sigma)^2(1/n^2-1/m^2)} = 1,44 \cdot 10^{-8}$ см, где $n = 2; m = 3$.

5.

37. $\mathscr{E} = h\nu = \mathrm{Ry}(Z-1)\left(\frac{1}{1^2} - \frac{1}{2^2}\right) \approx 17,15$ кэВ; $\nu \approx 4,14 \cdot 10^{18}\Gamma, \lambda_\alpha \approx \approx 0,072$ нм. Из экспериментальных данных известно, что для $20 < Z < 30$ постоянная экранирования $\sigma_{\text{экр}} = 1,13$.

5.

38. Чтобы появилась линия K_α нужно выбить электрон из K-оболочки. В грубом приближении для этого требуется ионизовать атом. При этом $eV = \mathrm{Ry}(Z-1)^2$. Таким образом, $V_{\text{Mo}} \approx 23$kB; $V_{\text{Cu}} \approx 10,6\kappa$B; $V_{\text{Fe}} \approx 8,5\kappa$B.

Эти результаты можно уточнить. Так, в атоме Mo структура незаполненных электронных оболочек $-4d^55s^1$, т. е. есть свободные места в $4d$-оболочке, откуда $eV_{\text{Mo}'} = \mathrm{Ry}(Z-1)^2\left(\frac{1}{1^2} - \frac{1}{4^2}\right) \approx 21,4$ кэВ. В атоме Cu структура

внешних электронных оболочек $-3d^{10}4s^1$, при этом в $3d$-оболочке мест нет и, следовательно, требуемый переход - в $4s$. Поэтому $V_{\text{Cu}} \approx 10$ кВ. Структура внешних электронных оболочек Fe $- 3d^64s^2$, откуда $V_{\text{Fe}} \approx 7,55$ кВ .

5.

39. Решение. K-полоса образуется при переходах K-электронов на свободные места. При таких переходах наиболее вероятно излучение электродипольных или El-фотонов. Самое коротковолновое излучение было бы при переходе внешнего электрона, т. е. $5s \to 1s$. Но такой переход с излучением $E1$-фотона является $(0-0)$-переходом и поэтому запрещен правилами отбора по L. Кроме того, для $E1$-фотона этот переход запрещен еще и по закону сохранения четности. Таким образом, границы K-серии соответствуют переходу $4p$-электрона (d-электроны не дают электродипольного излучения, потому что $\Delta L = 2$). Возможные и запрещен-

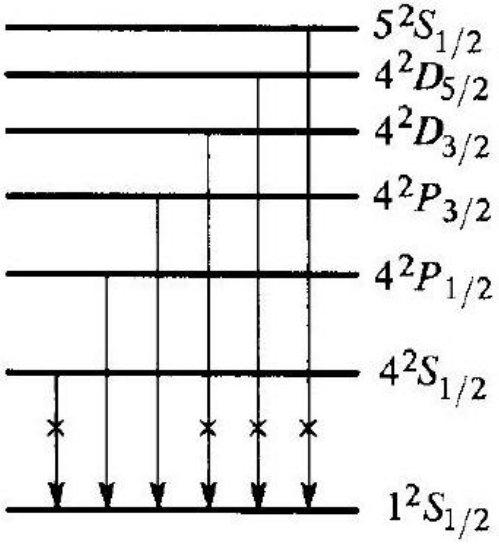


Рис. 159 ные переходы изображены на рис. 159. Пренебрегая расщеплением уровней из-за спин-орбитального расщепления, получаем

$$\frac{hc}{\lambda_{\text{гр}}} = \text{Ry}(Z-1)^2\left(\frac{1}{1^2}-\frac{1}{4^2}\right)$$

откуда $\lambda_{\text{гр}} = 5,79\cdot 10^{-9}$ см $\approx 0,058$ нм.
Для атома меди (Cu) с конфигурацией электронных оболочек $1s^22s^22p^63s^23p^63d^{10}4s^1$ границы соответствуют переходу $3p$-электрона

$$\lambda_{гр} \approx 0,013$$

Для атома железа (Fe) конфигурация электронной оболочки имеет вид $1s^22s^22p^63s^23p^63d^64s^2$ - все аналогично меди

$$\lambda_{\text{гр}} = 1,64\cdot 10^{-9}\text{с} \approx 0,016\text{Н}$$

5.

40. Электронная конфигурация атома Co $1s^22s^22p^63s^23p^63d^74s^2$. Учитывая, что для этого атома переход $4s-1s$ с излучением $E1$-фотона запрещен, $\mathscr{E}^{\text{Co}}_{K_{\text{гр}}} \approx 8,172$ кэВ. Минимальная энергия для возбуждения K-излучения Ni(линия K_α) есть $\mathscr{E}^{\text{Ni}}_{K_\alpha} \approx 8,813$ кэВ. Поскольку $\mathscr{E}^{\text{Ni}}_{K_\alpha} > \mathscr{E}^{\text{Co}}_{K_{\text{гр}}}$, то K-серия атома Ni не возбуждается. Остальные линии - возбуждаются.

5.

41. Zr и Mo; между ними находится элемент Nb .

5.

42. Na ($3S \to 2P$-переходы).

5.

43. $V = 15\kappa B$.

5.

49. $T = -\frac{\hbar^2}{k\mu d^2\ln(\alpha/3)} = 1,4$ K. Здесь отношение заселенностей состояний записано с учетом их статистических весов (кратностей вырождения): $\alpha = \frac{N(l_1=1)}{N(l_2=0)} = \frac{2l_1+1}{2l_2+1}\exp\left(-\frac{\mathscr{E}(l_1)-\mathscr{E}(l_2)}{kT}\right) = 3\exp\left(-\frac{\hbar^2}{kTI}\right)$.

5.

50. $\frac{\Delta\lambda}{\lambda} = \frac{\Delta\mu}{\mu} = 2,5\cdot 10^{-2}$, где μ - приведенная масса молекулы. Наибольшей длине волны соответствует переход из $l=1$ в $l=0$, откуда $\lambda = 2,65$ мм .

5.

51. $\frac{\Delta\lambda}{\lambda} = \frac{\Delta\mu}{2\mu} = 7,7\cdot 10^{-4}$, где μ - приведенная масса молекулы.

5.

52. $w(0) = \frac{2}{\pi\sqrt{2n}} = 0,14.$

$$\int^{x_0} e^{-x^2/x_0^2} dx$$

5.

53. $w = \frac{-x_0}{\infty} \approx 0,865.$

$$\int_{-\infty}^{\infty} e^{-x^2/x_0^2} dx$$

5.

54. $l_{\max} \approx \left[\sqrt[4]{\frac{4M_{\text{а3}}}{m_{\text{e}}}}\right] + 1 = 18$, где $M_{\text{а3}}$ - масса атома азота, m_{e} масса электрона. Квадратные скобки здесь и в следующей задаче означают операцию взятия целой части числа.

5.

55. $N_{\max} = [n_{\max}] + 1 = 81$, где $n_{\max} = \frac{1-\alpha}{2\alpha} \approx 80,9.$

5.

56. $\delta\mathscr{E}_{205} - \delta\mathscr{E}_{203} = \delta\mathscr{E}_{203}\frac{2}{3}\frac{\Delta A}{A} \approx 0,05$ эВ. Тогда $\delta\mathscr{E}_{205} = \delta\mathscr{E}_{203} + 0,05 = -8,2$ эВ (энергия ионизации в атоме с ядром ^{205}Tl меньше, чем в атоме с ядром ^{203} T1).

5.

57: $\frac{\Delta\omega}{\omega_0} = -0,046.$
Решение. Гамильтониан относительного движения атомов в молекуле имеет вид

$$\widehat{H} = -\frac{\hbar^2}{2\mu}\Delta_r + \frac{\hbar^2 l(l+1)}{2\mu r^2} + \frac{\varepsilon\sigma^2}{r^2} - 2\frac{\varepsilon\sigma}{r}$$

где $\Delta_r = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}$ - радиальная часть лаплассиана, $\mu = \frac{m_{\text{H}} m_{\text{Cl}}}{m_{\text{H}} + m_{\text{Cl}}} \approx m_{\text{H}}$ - приведенная масса. Следовательно, эффективный потенциал

$$U(r) = U_{\text{цбеж}}(r) + U(r) = \frac{A_l}{r^2} - \frac{B}{r}$$

где $A_l = \frac{\hbar^2 l(l+1)}{2\mu} + \varepsilon\sigma^2 = \varepsilon\sigma^2\left[1 + \frac{\hbar^2 l(l+1)}{2\mu\varepsilon\sigma^2}\right] = \varepsilon\sigma^2(1+\delta_l), B = 2\varepsilon\sigma$. Минимум эффективного потенциала находится при $r_0 = \frac{2A_l}{B}$. Раскладывая потенциал вблизи минимума

$$U_{\text{Эфф}}(r) \simeq U_\phi(r_0) + \frac{1}{2}\frac{d^2 U_{\text{эфф}}}{dr^2}\bigg|_{r=r_0}(r-r_0)^2,$$

получаем выражение для коэффициента жесткости

$$k = \frac{1}{2}\frac{d^2 U_{\text{эфф}}}{dr^2}\bigg|_{r=r_0} = \frac{B^4}{8A_l^3}.$$

Частота колебаний $\omega_l = \sqrt{\frac{k}{\mu}} = \left(\frac{B}{A_l}\right)^2\sqrt{\frac{A_l}{8\mu}}$.
Поскольку $\delta_l = \frac{\hbar^2 l(l+1)}{2\mu\varepsilon\sigma^2} = 0,024 \ll 1$, то

$$\omega_l \approx \frac{4}{\sigma^2}(1-2\delta_l)\sqrt{\frac{\varepsilon\sigma^2}{8\mu}}\left(1+\frac{\delta_l}{2}\right) \approx \sqrt{\frac{2\varepsilon}{\mu\sigma^2}}\left(1-\frac{3}{2}\delta_l\right).$$

Введем обозначение $\omega_0 = \sqrt{\frac{2\varepsilon}{\mu\sigma^2}}$ - частота колебаний в основном состоянии.
Тогда

$$\omega_l = \omega_0\left(1-\frac{3}{2}\delta_l\right) \text{ и } \frac{\Delta\omega}{\omega} = -\frac{3}{2}\delta_l = -0,046.$$

См. также решение задачи 5.31.
Заметим, что квант колебаний $\hbar\omega_0 = \sqrt{2\varepsilon\frac{\hbar^2}{\mu\sigma^2}} = 0,146$ эВ. Равновесное расстояние между атомами $r_0 \approx \alpha$.

Если ввести обозначения $\frac{\hbar^2 l(l+1)}{2\mu r^2} + \frac{\varepsilon\sigma^2}{r^2} = \frac{\hbar^2 l^*(l^*+1)}{2\mu r^2}$ и $2\varepsilon\sigma = (l^*)^2$, то получим гамильтониан атома водорода. Используя известный результат, получаем полную энергию молекулы $\mathscr{E} = -\frac{\mu(e^*)^4}{2\hbar^2}\frac{1}{(n_r+l^*+1)^2}$. Если $n_r,\, l \ll \frac{2\mu\varepsilon\sigma^2}{\hbar^2}$, то полученную формулу можно разложить в ряд и получить

$$\mathscr{E} = -\varepsilon + \hbar\sqrt{\frac{2\varepsilon}{\mu\sigma^2}}\left(n_r+\frac{1}{2}\right) + \frac{\hbar^2}{2\mu\sigma^2}\left(l+\frac{1}{2}\right)^2 - \\ - \frac{3\hbar^2}{2\mu\sigma^2}\left(n_r+\frac{1}{2}\right)^2 - \frac{3\hbar^3}{2\mu^2\sigma^4}\sqrt{\frac{\mu\sigma^2}{2\varepsilon}}\left(n_r+\frac{1}{2}\right)\left(l+\frac{1}{2}\right).$$

Первые три члена этой формулы соответствуют электронной, колебательной и вращательной энергиям молекулы (задача 5.29). Четвертый член соответствует ангармонизму колебаний (задача 5.55), а пятый - взаимодействию колебаний и вращений ядер (задачи 5.31 и 5.57). Не смотря на свою простоту, которая позволяет получить аналитическое решение, потенциал Кратцера плохо описывает реальную форму потенциала взаимодействия: на малых расстояниях отталкивание атомов в молекулах сильнее, а на больших расстояниях - притяжение слабее. Поэтому в теории молекул обычно используют потенциал Морса (задача 5.33), а в конденсированных средах потенциал Леннарда-Джонса.

20.4 Many-Body Quantum Mechanics Problems

20.4.1 Problems about Addition of Momenta and Particle Identity

(потом быстро мб потренируюсь, пропишу теорию про это! сложение моментов и операторы дискретных симметрий. тут еще подумать нужно про это!)

Б-2.10.1 Суммарный спин системы с двумя электронами

Найти собственные значения и собственные функции операторов $\hat{\mathbf{S}}^2$ и $\hat{\mathrm{S}}_z$ системы двух электронов $\left(\hat{\mathbf{S}} = \hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2\right)$, $s_i = 1/2$. Установить связь перестановочной симметрии спиновой функции с суммарным спином S.

Обозначим одночастичные спиновые функции $\chi_{1/2}(1,2)$, $\chi_{1/2}(2)$ и $\chi_{-1/2}(1)$, $\chi_{-1/2}(2)$ где цифры 1,2 нумеруют частицы. Должны выполняться условия

$$\hat{s}_{1z}\chi_{1/2}(1) = +\frac{1}{2}\chi_{1/2}(1),$$

$$\hat{s}_{2z}\chi_{1/2}(2) = +\frac{1}{2}\chi_{1/2}(2),$$

$$\hat{s}_{1,2z}\chi_{-1/2}(1) = -\frac{1}{2}\chi_{-1/2}(1),$$

$$\hat{s}_{1,2z}\chi_{-1/2}(2) = -\frac{1}{2}\chi_{-1/2}(2).$$

где $\hat{s}_{1z}, \hat{s}_{2z}$ - одночастичные спиновые операторы, действующие только на спиновые функции 1-й или 2-й частицы. Для волновой функции с суммарным спином ψ_{SM} выполняется

$$\hat{\mathbf{S}}^2\psi_{SM} = S(S+1)\psi_{SM},$$
$$\hat{S}_z\psi_{SM} = M\psi_{SM},$$

где $\hat{\mathbf{S}} = \hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2$ - оператор суммарного спина.

Находим старший и младший вектор - собственные функции операторов $\hat{\mathbf{S}}^2$ и $\hat{\mathrm{S}}_z$, отвечающие собственным значениям $S = 1, M = \pm 1$. Эти вектора реализуются, если обе частицы имеют спин или только в одну или только в противоположную сторону:

$$\psi_{1,1} = \chi_{1/2}(1)\chi_{1/2}(2),$$
$$\psi_{1,-1} = \chi_{-1/2}(1)\chi_{-1/2}(2).$$

Действуем на старший вектор $\psi_{1,1}$ понижающим оператором S_-, которым воспользуемся, представив его как $\hat{\mathrm{S}}_- = \hat{\mathrm{s}}_{1-} + \hat{\mathrm{s}}_{2-}$. После действия его получатся функция с $M = 0$:

$$\psi_{1,0} = \frac{1}{\sqrt{2}}\left(\chi_{1/2}(1)\chi_{-1/2}(2) + \chi_{-1/2}(1)\chi_{1/2}(2)\right).$$

и также она же получается, если подействовать по формуле $J_-|J, M\rangle = \sqrt{J(J+1) - M(M-1)}|J, M-1\rangle$. То есть мы вывели, что $|j^A + j^B, j^A + j^B - 1\rangle = \sqrt{\frac{j^A}{j^A+j^B}}|j^A, j^A - 1\rangle|j^B, j^B\rangle + \sqrt{\frac{j^B}{j^A+j^B}}|j^A, j^A\rangle|j^B, j^B - 1\rangle$.

Из вида вектора $\psi_{1,0}$ заключаем, что он имеет один ортогональный. Выберем его как

$$\psi_{1,0\perp} = \frac{1}{\sqrt{2}}\left(\chi_{1/2}(1)\chi_{-1/2}(2) - \chi_{-1/2}(1)\chi_{1/2}(2)\right).$$

Ортогональность очевидна, а коэффициент вначале находится из нормировки. Подействовав на него повышающим оператором $S_+ = s_{1+} + s_{2+}$, где каждый действует как $j_\pm|j, m\rangle = \sqrt{j(j+1) - m(m \pm 1)}|j, m \pm 1\rangle$, видим, что он обращается в ноль, таким образом, для $M = 0$ мы имеем старший вектор, то есть

$$\psi_{0,0} = \frac{1}{\sqrt{2}}\left(\chi_{1/2}(1)\chi_{-1/2}(2) - \chi_{-1/2}(1)\chi_{1/2}(2)\right).$$

Спиновые функции ψ_{SM} обладают определенной симметрией по отношению к перестановкам спиновых переменных $1 \leftrightarrow 2$: они симметричны при $S = 1$ и антисимметричны при $S = 0$.

Об операторе спинового обмена (??)

(не понял, как им пользоваться пока что.)

Заметим в этой связи, что для нахождения функций ψ мм можно было бы воспользоваться оператором спинового обмена $\hat{\mathrm{P}}_{12}$. Он действует на спиновые функции следующим образом: $\hat{\mathrm{P}}_{12}\psi_{SM}(1, 2) = \psi_{SM}(2, 1)$, т. е. как раз переставляет спиновые переменные. Оператор $\hat{\mathrm{P}}_{12}$ коммутирует с $\hat{\mathbf{S}}^2$ и $\hat{\mathrm{S}}_2$, а поэтому искомые функции должны быть и его собственными функциями: $\hat{\mathrm{P}}_{12}\psi_{SM}(1, 2) = \lambda\psi_{SM}(1, 2)$. Легко видеть, что $\lambda = \pm 1$, а собственные функции должны быть симметричными ($\lambda = 1$) или антисимметричными ($\lambda = -1$). Поэтому можно сразу составить из одночастичных функций симметричные и антисимметричные комбинации, и тогда останется только определить значения квантовых чисел S и M.

Б-2.10.2 Элементарное сложение моментов

Найти собственные значения и собственные функции операторов $\hat{\mathbf{l}}^2$ и $\hat{\mathrm{l}}_z$ системы двух частиц с орбитальными моментами $l_1 = l_2 = 1$ $\left(\hat{\mathbf{l}} = \hat{\mathbf{l}}_1 + \hat{\mathbf{l}}_2\right)$. Воспользоваться соотношениями ортогональности для коэффициентов Клебша-Гордана. Определить связь между квантовым числом суммарного момента L и перестановочной симметрией координатной волновой функции.

Б-2.10.3 Элементарное сложение моментов

Найти собственные значения и собственные функции операторов $\hat{j}^2$ и $\hat{j}_z$ частицы со спином 1/2 в случае, когда орбитальное квантовое число равно $l(\hat{\mathbf{j}} = \hat{I} + \hat{\mathbf{s}})$.

(У киселева решена, соберу потом сюда решение тоже!)

Б-2.10.4 Средние значения операторов частицы в атоме водорода (??)

Вычислить средние значения операторов $(\hat{I}\hat{\mathrm{s}})$, $(\hat{\mathrm{j}})$ и $(\hat{\mathrm{j}}\hat{\mathrm{s}})$ в состоянии $|l, s, j, m_j\rangle$.

(?? что за операторы???)

Б-2.10.5 Оператор обмена спинами (!?!??)

Показать, что оператор $\hat{\mathrm{P}}_{12} = \frac{1}{2}(1 + \hat{\boldsymbol{\sigma}}_1\hat{\sigma}_2)$ является оператором обмена спинами, т. е. $\hat{\mathrm{P}}_{12}\hat{\boldsymbol{\sigma}}_1\hat{\mathrm{P}}_{12}^{-1} = \hat{\boldsymbol{\sigma}}_2$.

Б-2.10.6 Ферми- и бозе- частицы в ящике

Найти уровни энергии и волновые функции стационарных состояний двух невзаимодействующих тождественных частиц в потенциальном ящике

$$V(x) = \begin{cases} 0, & 0 < x < a \\ \infty, & x < 0, x > a \end{cases}$$

если этими частицами являются:
а) ферми-частицы со спинами $s = 1/2$;
б) бозе-частицы со спинами $s = 0$;
в) бозе-частицы со спинами $s = 1$.
Чему равна в каждом из этих случаев энергия основного состояния N частиц?
(??? тупая задача, неужели суть её в том, что не важно, ферми и бозе ли частицы у нас?)
Одночастичные координатные функции и уровни энергии имеют вид

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin \frac{\pi n}{a} x, & 0 < x < a, \\ 0, & x \leqslant 0, x \geqslant a, \end{cases} \qquad E_n = \frac{\hbar^2 k^2}{2m} = \frac{\pi^2 \hbar^2}{2ma^2} n^2.$$

а) Ферми-частицы со спином $1/2$. Полная волновая функция Ψ (произведение координатной и спиновой функций) должна быть антисимметричной, поэтому в случае $n_1 \neq n_2$ возможны два варнанта:

$$\Psi_{n_1 n_2} = \psi_A(x_1, x_2)\, \chi_S(S, M) \quad \text{и} \quad \Psi_{n_1 n_2} = \psi_S(x_1, x_2)\, \chi_A(S, M),$$

где ψ_A и ψ_S - антисимметричная и симметричная комбинации одночаные в задаче 2.10.1. Таким образом, х отвечает значению суммарного спина $S = 0$ (одна функция), а \ s отвечает состояниям с $S = 1$ (три функции). Энергия состояния двух частиц $E_{n_1 n_2} = \frac{\pi^2 \hbar^2}{2ma^2} \left(n_1^2 + n_2^2\right)$.

В случае $n_1 = n_2 = n$ может реализоваться только симметричная координатная функция ψ_S, поэтому спиновая функция должна быть антисимметричной: χ A, т. е. такому состоянию отвечает значение $S = 0$. Энергия состояня двух частиц равна $E_{nn} = \frac{\pi^2 \hbar^2}{ma^2} n^2$. Энергия основного состояния N частиц:

$$E = \begin{cases} \frac{\pi^2 \hbar^2}{24ma^2} N(N+1)(N+2), & \text{если } N = 2n \\ \frac{\pi^2 \hbar^2}{24ma^2} (N+1)\left(N^2 + 2N + 3\right), & \text{если } N = 2n+1 \end{cases}$$

б) Бозе-частицы со спином 0. Полная волновая функция (она же - координатная) может быть только симметричной:

$$\Psi_{n_1 n_2} = \psi_S(x_1, x_2) = \frac{1}{\sqrt{2}} \left[\psi_{n_1}(x_1)\, \psi_{n_2}(x_2) + \psi_{n_1}(x_2)\, \psi_{n_2}(x_1)\right]$$

Энергия двух частиц: $E_{n_1 n_2} = \frac{\pi^2 \hbar^2}{2ma^2} \left(n_1^2 + n_2^2\right)$.

в) Бозе-частицы со спином 1. Полная волновая функция Ψ (произведение координатной и спиновой функций) должна быть симметричной, поэтому возможны два варианта ($n_1 \neq n_2$):

$$\Psi_{n_1 n_2} = \psi_S(x_1, x_2)\, \chi_S(S, M) \text{ и } \Psi_{n_1 n_2} = \psi_A(x_1, x_2)\, \chi_A(S, M),$$

где спиновые функции имеют точно такой же вид, как и общие собственные функции операторов $\hat{\mathbf{L}}^2$ и $\hat{l}_z$ из решения задачи 2.10.2. Следоа χ_S отвечает состояниям с $S = 0, 2$ (шесть функций). Энергия двух частиц: $E_{n_1 n_2} = \frac{\pi^2 \hbar^2}{2ma^2} \left(n_1^2 + n_2^2\right)$.

В случае $n_1 = n_2 = n$ может реализоваться только симметричная координатная функция ψ_s, поэтому спиновая функция должна быть также симметричной: χS, т. е. такому состоянию отвечают значения $S = 0, 2$.

Энергия основного состояния N частиц для случаев б) и в) одинакова и равна

$$E = \frac{\pi^2 \hbar^2}{2ma^2} N$$

Б-2.10.7 Распад на две альфа-частицы ядра с $J = 1$

Может ли распасться на две альфа-частицы нестабильное ядро $^8\mathrm{Be}^*$, находящееся в состоянии с $J = 1$?

Спин α-частиц равен нулю, и их общая волновая функция должна быть симметрична по отношению к перестановкам пространственных переменных. В системе центра масс такая перестановка приводит к преобразованию $\mathbf{r} \to -\mathbf{r}$, где $\mathbf{r}$ - относительная координата.

Для определения вида волновой функции нам может понимание P-четности. При зеркальном отражении всех осей евклидова пространства $\boldsymbol{r} \xrightarrow{\hat{P}} -\boldsymbol{r}$ углы преобразуются как

$$\phi \xrightarrow{\hat{P}} \phi + \pi, \quad \theta \xrightarrow{\hat{P}} \pi - \theta,$$

или

$$e^{im\phi} \xrightarrow{\hat{P}} e^{im(\phi+\pi)} = (-1)^m e^{im\phi}, \quad \cos\theta \xrightarrow{\hat{P}} -\cos\theta.$$

Присоединенные полиномы Лежандра суть производные функции четности $(-1)^l$, так что их четность определяется просто числом производных, и

$$P_{l,m}(\cos\theta) \xrightarrow{\hat{P}} (-1)^{l-m} P_{l,m}(\cos\theta).$$

Собирая факторы, находим

$$y_{l,m}(\theta,\phi) \xrightarrow{\hat{P}} (-1)^l y_{l,m}(\theta,\phi).$$

Другими словами, P-четность сферических гармоник равна

$$\lambda_P = (-1)^l.$$

То есть при данной замене угловая часть волновой функции α-частиц должна умножаться на $(-1)^L$ - четность состояния (L - полный орбитальный момент). Число L должно быть четным, потому что волновая функция симметрична. Поэтому и полный момент ядра Be также должен быть четным. Следовательно, при $J = 1$ распад невозможен.

20.4.2 Simple Problems of Solid State Physics

(если это не простейшее - в физику твердого тела занесу)

простейшие одномерные модели

Модели типа Кронига-Пенни

мотивация

если Пироженко ей занималась, значит, все-таки что-то есть в этом.
наверное, там много моделей.

типичная модель

(задача из Белоусова)

ЛШ-1 Классическая цепочка осцилляторов

итоговые свойства

описание модели

Рассмотрим цепочку атомов массы m_i, соединенньх одинаковыми пружинками жесткости K:

$$\mathcal{H} = \sum_{i=-\infty}^{\infty} \left[p_i^2/(2m_i) + (K/2)(x_i - x_{i+1})^2 \right]$$

где $m_i = m$, если i четно, и $m_i = M$, если i нечетно.

1. Определите нормальные моды для этой системы. Покажите, что их две: акустическая и оптическая.

2. Чему равна скорость звука c? Получится ли такой же ответ, если вычислять c по формуле Лапласа $c = \sqrt{\partial P/\partial\rho}$, где P -давление, а ρ -плотность?

3. Чему равна ширина щели между оптической и акустической ветвями? Покажите, что при $M \gg m$ дисперсия оптической моды практически отсутствует. Как можно объяснить это качественно?

решение модели

$$m\ddot{x}_i = K\left(y_i + y_{i-1} - 2x_i\right), \quad M\ddot{y}_i = K\left(x_i + x_{i+1} - 2y_i\right)$$

(x_i - смещение атома массы m в i -й элементарной ячейке, y_i -смещение атома массы M).

Будем искать решение в виде плоских волн:

$$x_n = e^{i(qn-\omega t)}x_q, \quad y_n = e^{i[q(n+1/2)-\omega t]}y_q$$

Отсюда

$$m\omega^2 x_q = 2Kx_q - 2K\cos(q/2)y_q, \quad M\omega^2 y_q = 2Ky_q - 2K\cos(q/2)x_q$$

(Здесь q -волновой вектор в первой зоне Бриллюэна: $-\pi < q < \pi$.) Нормальные моды имеют закон дисперсии, определяемый из условия

$$\det\begin{pmatrix} 2K - m\omega^2 & -2K\cos(q/2) \\ -2K\cos(q/2) & 2K - M\omega^2 \end{pmatrix} = 0$$

что дает $\omega^4 - (2K/\mu)\omega^2 + \left(4K^2/mM\right)\sin^2(q/2) = 0$, где $\mu = Mm/(M+m)$.

Получаем

$$\omega_{\pm}^2(q) = \frac{K}{\mu}\left(1 \pm \sqrt{1 - \frac{4\mu^2}{mM}\sin^2(q/2)}\right)$$

Здесь «+» соответствует оптической, а «-» - акустической моде.

Дисперсия нормальных мод (1.27) показана на рис. 1.1.

(вставлю, типичный рисунок)

При малых q разлагаем закон дисперсии акустической моды:

$$\omega_-^2(q) = \frac{2K\mu}{mM}(q/2)^2$$

и получаем скорость звука:

$$c = \left(\omega_-/q\right)|_{q\to 0} = \frac{1}{2}(2K/(M+m))^{1/2}$$

При выводе предполагалось, что период решетки $2a$ равен единице.

Чтобы получить выражение, имеющее размерность скорости, надо умножить результат на $2a$, где a -расстояние между атомами M и m.

При этом получается скорость $c = a\sqrt{2K/(M+m)}$ Проверим, что найденная скорость звука согласуется с формулой Лапласа $c^2 = \partial P/\partial\rho$, связываюшей скорость звука и сжимаемость системы.

Для цепочки длины x, содержашей N атомов каждого типа, сила пропорциональна удлинению, $dP = -(K/2N)dx($ в одном измерении сила и давление - это одно и то же), а изменение плотности есть

$$d\rho = \frac{d}{dx}\left(\frac{(M+m)N}{x}\right)dx = -\frac{(M+m)N}{x_0^2}dx$$

где $x_0 = 2$ Na.

Отсюда получаем $c^2 = 2\mathrm{Ka}^2/(M+m)$, как и следовало.

Верхний край акустической ветви спектра:

$$\max\left[\omega_-^2(q)\right] = \omega_-^2(\pi) = \frac{K}{\mu}\left(1 - \sqrt{1 - \frac{4\mu^2}{mM}}\right) = \frac{K}{\mu}\left(1 - \frac{M-m}{M+m}\right) = \frac{2K}{M}$$

Аналогично, нижний край оптической ветви есть

$$\min\left[\omega_+^2(q)\right] = \omega_+^2(\pi) = \frac{2K}{m}$$

и поэтому ширина щели $\Delta\omega = \sqrt{2K/m} - \sqrt{2K/M}$.

При $M \gg m$ частота оптической ветви

$$\omega_+(q) = \sqrt{\frac{2K}{m}}\left(1 + \frac{m}{2M}\cos^2(q/2) + O\left(\frac{m^2}{M^2}\right)\right)$$

практически не зависит от q, что соответствует колебаниям легких атомов между почти неподвижными тяжелыми.

Физическая причина отсутствия дисперсии - взаимная независимость колебаний соседних атомов массы m.

При $M \gg m$ неважно, колеблются ли соседние легкие атомы в фазе или же в противофазе, поскольку через тяжелые стенки (т.е.

атомы массы M) влияние не передается.

ЛШ-2 Фермионная цепочка

итоговые свойства

обзор и применения

хз зачем нужна.

описание модели

Найдите преобразование Боголюбова, диагонализующее фермионный гамильтониан

$$\hat{\mathcal{H}} = \sum_{i=-\infty}^{\infty} \left(J_1 a_i^+ a_{i+1} + J_1 a_{i+1}^+ a_i + J_2 a_i a_{i+1} + J_2 a_{i+1}^+ a_i^+ - 2B a_i^+ a_i \right)$$

Такой гамильтониан возникает при рассмотрении одномерной модели квантового магнетика, так называемой «XY-модели»
(см. раздел 1.4).
Определите спектр квазичастиц $\varepsilon(k)$ этого гамильтониана.
Обратите внимание, что при $B = 0$ и $J_1 = J_2$ дисперсия пропадает.
Можно ли понять это без вычислений?

решение 1

Сделаем преобразование Фурье $a_m = \int\limits_{-\pi}^{\pi} e^{ikm} a_k \frac{dk}{2\pi}$.

При этом члены гамильтониана преобразуются к такому виду:

$$\sum_m a_m^+ a_{m+1} = \sum_k a_k^+ a_k e^{ik}, \sum_m a_m a_{m+1} = \sum_k a_k a_{-k} e^{-ik}$$
$$\sum_m a_m^+ a_{m+1} + a_{m+1}^+ a_m = \sum_k 2\cos k a_k^+ a_k$$

где сумма по k есть сокращенное обозначение для $\int\limits_{-}^{\pi} \ldots \frac{dk}{2\pi}$.

Пользуясь антикоммутативностью a_k и a_{-k}, перепишем вторую сумму так:

$$\sum_m a_m a_{m+1} = -i \sum_k \sin k a_k a_{-k}$$

после чего гамильтониан принимает вид

$$\hat{\mathcal{H}} = \sum_k \left(2\left(J_1 \cos k - B\right) a_k^+ a_k - i J_2 \sin k a_k a_{-k} + i J_2 \sin k a_{-k}^+ a_k^+ \right)$$

После «поворота» $a_k = e^{i\pi/4} b_k, a_k^+ = e^{-i\pi/4} b_k^+$ гамильтониан становится вещественным:

$$\hat{\mathcal{H}} = \sum_k \left(\left(J_1 \cos k - B\right) b_k^+ b_k + J_2 \sin k b_k b_{-k} + \text{ h.c} \right)$$

Будем искать фермионное преобразование Боголюбова в виде

$$b_k = u_k c_k + v_k c_{-k}^+, \qquad b_k^+ = u_k c_k^+ + v_k c_{-k}$$
$$b_{-k}^+ = -v_k c_k + u_k c_{-k}^+, \quad b_{-k} = -v_k c_k^+ + u_k c_{-k}$$

с вещественными u_k и v_k, причем $u_k^2 + v_k^2 = 1$.
Получаем

$$\hat{\mathcal{H}} = \sum_k \left(J_1 \cos k - B\right) \left(u_k^2 c_k^+ c_k + u_k v_k \left(c_k^+ c_{-k}^+ + c_{-k} c_k \right) + v_k^2 c_{-k} c_{-k}^+ \right) +$$
$$+ J_2 \sin k \left(u_k^2 c_k c_{-k} + u_k v_k \left(c_{-k}^+ c_{-k} - c_k c_k^+ \right) - v_k^2 c_{-k}^+ c_k^+ \right) + \text{h.c}$$

Приравняем коэффициент при $c_{-k}c_k$ нулю, потребовав чтобы

$$2u_kv_k\left(J_1\cos k - B\right) + \left(-u_k^2 + v_k^2\right)J_2\sin k = 0$$

Тогда будем иметь слкдующее

$$\frac{v_k}{u_k} = \frac{B - J_1\cos k \pm \sqrt{\left(J_1\cos k - B\right)^2 + J_2^2\sin^2 k}}{J_2\sin k}$$

Решив это уравнение при условии $u_k^2 + v_k^2 = 1$, найдем значения u_k, v_k и подставим их в гамильтониан:

$$\hat{\mathcal{H}} = \text{const} + \sum_k \left[2\left(J_1\cos k - B\right)\left(u_k^2 - v_k^2\right) + 4J_2\sin k u_k v_k\right] c_k^+ c_k =$$

$$= \text{const} + \sum_k \varepsilon_k c_k^+ c_k$$

Спектр возбуждений, таким образом, есть

$$\varepsilon_k = 2\sqrt{\left(J_1\cos k - B\right)^2 + J_2^2\sin^2 k}$$

Отсутствие дисперсии при $J_1 = J_2$ и $B = 0$ означает, что возбуждения локализованы на одном или нескольких соседних узлах.

Это можно понять с точки зрения преобразования Йордана-Вигнера (см.
раздел 1.4), которое в данном случае приводит к изинговской спиновой цепочке:

$$\hat{\mathcal{H}} = \sum_{i=-\infty}^{\infty} J_y\sigma_i^y\sigma_{i+1}^y$$

В такой цепочке каждый спин характеризуется определенной проекцией на ось y.

Поэтому элементарное возбуждение в этой системе - просто переворот спина на любом из узлов, никак не затрагивающий остальные узлы.

Таким образом, полная локализация возбуждения на одном узле эквивалентна отсутствию дисперсии.

Обратим внимание на аналогию с задачей 1 в случае $M \gg m$ когда оптическая мода колебаний становится почти бездисперсионной из-за того, что колебания соседних легких атомов почти полностью развязаны.

второе решение

не актуально к сожалению.

ЛШ-3 Нелинейные канонические преобразования

итоговые свойства

описание модели

Рассмотрим фермиевские операторы a и a^+, действующие в пространстве состояний фермиона, который может заполнять или не заполнять ровно одно состояние.

В этом случае пространство многочастичных состояний двумерно и каноническим базисом в нем служат состояния $|0\rangle$ и $|1\rangle$.

Найдите все канонические преобразования операторов a и a^+, сохраняющие соотношения $a^2 = \left(a^+\right)^2 = 0$ и $a^+a + aa^+ = 1$.

Убедитесь в том, что канонические преобразования наиболее общего вида не описываются линейными соотношениями вида (1.11).

Рассмотрите представление фермиевских операторов спиновыми матрицами Паули:

$$\sigma_x = a + a^+, \quad \sigma_y = i\left(a - a^+\right), \quad \sigma_z = 2a^+a - 1$$

Покажите, что канонические преобразования a и a^+ соответствуют вращениям в спиновом пространстве.

Связь между фермиевскими операторами и операторами спина 1/2 более подробно рассмотрена в разделе 1.4.

решение

Решение 3.
Будем искать каноническое преобразование в таком виде:

$$a' = ua + va^+ + wa^+a + q$$
$$a'^+ = u^*a^+ + v^*a + w^*a^+a + q^*$$

Это наиболее общая форма, к которой может быть приведено любое полиномиальное по a и a^+ выражение.
Убедиться в этом можно следующим образом.
Во-первьх, помощью коммутационньх соотношений любое выражение может быть приведено к нормальной форме, в которой в каждом слагаемом оператор a^+(если он есть) стоит слева от a.

Во-вторых, поскольку $a^2 = (a^+)^2 = 0$, выражение (1.56) представляет собой нормальную форму наиболее общего вида.
Рассмотрим выражение a'^2.
Приведем квадрат правой части выражения (1.56) для a' к нормальной форме и потребуем, чтобы все коэффициенты обратились в нуль.
Это дает два условия:

$$w + 2q = 0, \quad uv + q^2 = 0$$

Аналогично, условие $a'a'^+ + a'^+a' = 1$ приводит к соотношению

$$|u|^2 + |v|^2 + 2|q|^2 = 1$$

Из полученных соотношений следует, что

$$|u| + |v| = 1$$

Таким образом, наиболее общее каноническое преобразование задается двумя комплексными параметрами u и v, удовлетворяющими условию (1.60).
Коэффициенты q и w определяются таким образом: $q = \pm i\sqrt{uv}, w = -2q$.
Нетрудно видеть, что в обшем случае каноническое преобразование нелинейное, поскольку коэффициент w не обращается в нуль.
Более того, линейными оказываются лишь тривиальные преобразования (с u или v равным нулю).
Решим теперь задачу другим способом, воспользовавшись представлением (1.21) фермиевских операторов через матрицы Паули.
Обратим соотношения (1.21):

$$a = (\sigma_x - i\sigma_y)/2, \quad a^+ = (\sigma_x + i\sigma_y)/2$$

Нетрудно проверить, что условия $a^2 = (a^+)^2 = 0, a^+a + aa^+ = 1$ эквивалентны соотношениям антикоммутативности для σ_i:

$$[\sigma_i, \sigma_j]_+ = 2\delta_{ij}$$

Преобразования, сохраняющие соотношения (1.62), можно записать в виде

$$\sigma_i' = R_{ij}\sigma_j$$

где R_{ij} -вещественная ортогональная матрица 3×3.
Поэтому канонические преобразования в данном случае образуют группу SO(3).

ЛШ-4 Квантовая цепочка осцилляторов

итоговые свойства

описание модели

(??? условие утеряно??)
Пусть теперь гамильтониан (1.19) определяет квантовую задачу, т.е.
$p_i = -i\hbar\partial/\partial x_i$.
Перейдите к бозонным операторам рождения и уничтожения:

$$\hat{x}_i = \sqrt{\frac{\hbar}{m_i\omega_i}}\frac{a_i + a_i^+}{\sqrt{2}}, \quad \hat{p}_i = \sqrt{\hbar m_i\omega_i}\frac{a_i - a_i^+}{i\sqrt{2}}$$

Первое решение

(ниже все понятно, нужно бы когда-то проделать, чтобы потренироваться, пока забил, потому что суть понятна.)

Выразим $\hat{\mathcal{H}}$ через a_i и a_i^+ по формулам (1.22), не определяя пока частоту ω_0:

$$\hat{\mathcal{H}} = \sum \left(\frac{p_i^2}{2m} + \frac{K}{2} (x_i - x_{i+1})^2 \right) = -\sum \left[\frac{\hbar\omega_0}{4} \left(a_i - a_i^+\right)^2 + \frac{K\hbar}{4m\omega_0} \left(a_i + a_i^+ - a_{i+1} - a_{i+1}^+\right)^2 \right] =$$
$$= \sum \left[\frac{\hbar\omega_0}{4} \left(a_i^+ a_i - a_i^2\right) + \frac{\hbar K}{4m\omega_0} \left((a_i - a_{i+1}) \left(a_i^+ - a_{i+1}^+\right) + (a_i - a_{i+1})^2 \right) + \text{h.c} \right]$$

(с точностью до константы, возникающей из-за коммутационных соотношений бозеоператоров).

(потом мб проверю, пока не проверял)

Выполним преобразование Фурье:

$$a_m = \int_{-\pi}^{\pi} a_k e^{ikm} \frac{dk}{2\pi} = \sum_k a_k e^{ikm}, \quad a_k = \sum_m a_m e^{-ikm}$$

При этом

$$a_i - a_{i+1} \to \left(1 - e^{ik}\right) a_k,$$
$$a_i^+ - a_{i+1}^+ \to \left(1 - e^{-ik}\right) a_k^+$$

Подставляя эти выражения в (1.64), получаем

$$\hat{\mathcal{H}} = \sum_k \left(p(k) a_k^+ a_k + q(k) a_k a_{-k} + \text{ h.c} \right)$$

где $p(k) = \frac{\hbar\omega_0}{4} + \frac{\hbar K}{2m\omega_0}(1 - \cos k)$, $q(k) = \frac{\hbar K}{2m\omega_0}(1 - \cos k) - \frac{\hbar\omega_0}{4}$.

Рассмотрим каноническое преобразование:

$$a_k = u_k b_k + v_k b_{-k}^+, \quad a_{-k}^+ = v_k b_k + u_k b_{-k}^+$$

где $u_k = \operatorname{ch} \lambda_k, v_k = \operatorname{sh} \lambda_k$.

Нетрудно проверить, что при преобразовании (1.69) гамильтониан сохраняет свой вид, причем $p(k)$ и $q(k)$ меняются так:

$$p'(k) = \operatorname{ch} 2\lambda_k p(k) + \operatorname{sh} 2\lambda_k q(k)$$
$$q'(k) = \operatorname{sh} 2\lambda_k p(k) + \operatorname{ch} 2\lambda_k q(k)$$

(???? пока не вижу, почему они так меняются???)

Подберем λ_k так, чтобы $q'(k)$ обратилось в нуль:

$$\operatorname{th} 2\lambda_k = -q(k)/p(k)$$

При этом $p'(k) = \sqrt{p^2(k) - q^2(k)} = \hbar\sqrt{K/m} \sin|k/2|$.

Обратим внимание на то, что частота ω_0, значение которой может быть произвольным, выпадает из выражения для $p'(k)$ (но не из выражения для λ_k!).

Диагонализованный гамильтониан имеет вид

$$\hat{\mathcal{H}} = \sum_k \left(p'(k) b_k^+ b_k + \text{h.c} \right) = \sum_k \omega(k) \left(b_k^+ b_k + \frac{1}{2} \right)$$

второе решение

не актуально

20.4.3 Simple Problems of Quantum Mechanics of Gases

(пока тут, потом перенесу мб в статфиз)

ЛШ-7. Элементарные свойства ферми газа через обход полюса

Выразите плотность n ферми-газа через функцию Грина $G(\varepsilon, p)$, воспользовавшись соотношением (2.12).

Вычислите интеграл и получите формулу $p_0^3 = 3\pi^2 n$ для импульса Ферми p_0.

Solution

Используем причинную функцию Грина

$$G_{\alpha\beta} = -i\langle \mathrm{T}\psi_\alpha(\mathbf{r}, t)\psi_\beta^+(\mathbf{r}', t')\rangle = \delta_{\alpha\beta}G,$$

введенную в (2.8). Плотность частиц с проекцией спина α есть

$$n_\alpha(\mathbf{r}, t) = \lim_{t'\to t+0}\langle\psi_\alpha^+(\mathbf{r}, t')\,\psi_\alpha(\mathbf{r}, t)\rangle = -iG_{\alpha\alpha}(\mathbf{r}' = \mathbf{r}, t' = t + 0)$$

(при $t' = t - 0$ из-за перестановки ψ и ψ^+получилось бы $n_\alpha - 1$, по определению функции Грина). В нашем случае система однородна, и G зависит только от разности $\mathbf{r} - \mathbf{r}'$ и $t - t'$. Поэтому переходим в фурье-представление:

$$n_\alpha = -i\lim_{\tau\to-0}\int G(\varepsilon, \mathbf{p})e^{-i\varepsilon\tau}\frac{d^3\mathbf{p}d\varepsilon}{(2\pi)^4} =$$

$$= -i\lim_{\tau\to-0}\int_0^\infty \frac{4\pi p^2 dp}{(2\pi)^3}\int_{-\infty}^{+\infty}\frac{d\varepsilon}{2\pi}\frac{e^{-i\varepsilon\tau}}{\varepsilon - \xi(p) + i\delta\,\mathrm{sign}\,(p - p_0)},$$

где $\tau = t - t', \xi(p) = \mathbf{p}^2/2m - E_F$. Контур интегрирования по ε замыкаем в верхней полуплоскости, поскольку $\tau < 0$. При этом при $p > p_0$ полюс не захвачен:

$$\int\frac{d\varepsilon}{2\pi}\frac{e^{-i\varepsilon\tau}}{\varepsilon - \xi(p) + i\delta} = 0$$

а при $p < p_0$ захвачен:

$$\int\frac{d\varepsilon}{2\pi}\frac{e^{-i\varepsilon\tau}}{\varepsilon - \xi(p) - i\delta} = ie^{-i\xi(p)\tau}.$$

Знак мнимой части $i\delta$ определяет, заполнено ли состояние с данным p. С учетом спиновой двойки

$$n = 2\int_0^{p_0}\frac{4\pi p^2 dp}{(2\pi)^3} = p_0^3/\left(3\pi^2\right),$$

откуда находим $p_0^3 = 3\pi^2 n$.

ЛШ-8. Ферми частицы на прямой и полупрямой

а) Для невзаимодействующих ферми-частиц на прямой найдите функцию Грина $G_{\alpha\beta}(\varepsilon, x, x')$

б) То же для ферми-частиц на полупрямой $x > 0$ с граничным условием $\psi|_{x=0} = 0$

в) (Осцилляции Фриделя.) В случае полупрямой покажите, что плотность ферми-газа, как функция расстояния до стенки, осциллирует. Чему равен период осцилляций?

Solution 8 a.

Найдем

$$G_{\alpha\beta}(\varepsilon, x, x') = -i\int e^{i\varepsilon\tau}\langle\mathrm{T}\psi_\alpha(x)\psi_\beta^+(x')\rangle d\tau,$$

где $\tau = t - t'$. В импульсном представлении

$$G_{\alpha\beta}(\varepsilon, p) = \frac{\delta_{\alpha\beta}}{\varepsilon - \xi(p) + i\delta\,\mathrm{sign}\,\varepsilon}, \quad \xi(p) = \frac{p^2}{2m} - E_F.$$

Поэтому

$$G_{\alpha\beta}(\varepsilon, x, x') = \int e^{ip(x-x')}G_{\alpha\beta}(\varepsilon, p)\frac{dp}{2\pi} = -2m\delta_{\alpha\beta}\int\frac{e^{ip(x-x')}}{(p - p_1)(p - p_2)}\frac{dp}{2\pi}.$$

Полюсы подинтегрального выражения

$$p_{1,2} = \pm\varkappa,$$

где $\varkappa = \sqrt{2m(\varepsilon + E_F + i\delta\,\mathrm{sign}\,\varepsilon)}$. Если $\varepsilon > 0$, то p_1 лежит в верхней полуплоскости, а p_2 - в нижней, а если $\varepsilon < 0$, то наоборот.

Solution 8 б.

В присутствии стенки функцию Грина $G^{(1)}$ находим с помощью метода изображений:

$$G^{(1)}_{\alpha\beta}(\varepsilon, x, x') = G_{\alpha\beta}(\varepsilon, x, x') - G_{\alpha\beta}(\varepsilon, x, -x'),$$

где G дается (2.75). Обосновать такой ответ можно так же, как и при использовании метода изображений в электростатике. В самом деле, $G^{(1)}_{\alpha\beta}$ удовлетворяет уравнению

$$(\varepsilon - \hat{\mathcal{H}})G^{(1)}_{\alpha\beta}(\varepsilon, x, x') = \delta(x - x')\,\delta_{\alpha\beta}$$

и граничному условию $G^{(1)}_{\alpha\beta}(\varepsilon, 0, x') = 0$, а переход к изображениям обычным образом заменяет граничное условие условием антисимметрии.

Solution 8 в.

Выразим плотность через функцию Грина, найденную в части):

$$n(x) = -i \lim_{\tau \to -0} \mathrm{Tr} \int G^{(1)}_{\alpha\beta}(\varepsilon, x, x) e^{-i\varepsilon\tau} \frac{d\varepsilon}{2\pi},$$

где Tr означает взятие следа. Суммируя по спинам, получаем

$$n(x) = -2i \lim_{\tau \to -0} \int \frac{e^{-i\varepsilon\tau}\left(1 - e^{-2ipx}\right)}{\varepsilon - \xi(p) + i\delta\,\mathrm{sign}\,\xi(p)} \frac{dpd\varepsilon}{(2\pi)^2}.$$

При интегрировании по ε, поскольку $\tau < 0$, замыкаем контур в верхней полуплоскости. Полюс захватывается при $\xi(p) < 0$, т. е. при $p^2/2m < E_F$. Находим

$$n(x) = -2i \int\limits_{p^2 < 2mE_F} \left(1 - e^{-2ipx}\right) \frac{2\pi i}{(2\pi)} dp.$$

Интегрируем по p:

$$n(x) = 2 \int\limits_{-p_0}^{p_0} \left(1 - e^{-2ipx}\right) \frac{dp}{2\pi} = \frac{1}{\pi}\left(2p_0 - \int\limits_{-p_0}^{p_0} e^{-2ipx} dp\right) =$$
$$= \frac{1}{\pi}\left(2p_0 - \frac{\sin 2p_0 x}{x}\right) = n_0\left(1 - \frac{\sin 2p_0 x}{2p_0 x}\right)$$

где n_0 - плотность вдали от стенки. (Коэффициент в (2.81) можно проверить, подсчитав плотность частиц квазиклассически: $n_0 L = 2\,(2p_0 L)\,/2\pi\hbar$.)

Плотность $n(x)$ обращается в нуль на стенке, а вдали осциллирует с периодом $\lambda_0 = \pi\hbar/p_0$

Рис. 2.1

Сравним среднее расстояние между электронами $d = n_0^{-1} = \pi\hbar/2p_0$ с периодом осцилляций λ_0 - они отличаются в два раза. Это отличие связано со спином электронов. Фермиевские коррелящии, приводящие к осцилляциям, имеются только для электронов с одинаковой проекцией спина. Плотность таких электронов есть $n_0/2 = \lambda_0^{-1}$, что как раз соответствует периоду осцилляций.

20.5 Problems of Other Parts

20.5.1 Typical Problems of Relativistic Quantum Mechanics

Б-2.9.1 Коммутирование в релятивистском случае

Выяснить, какие из указанных ниже операторов коммутируют с гамильтонианом свободной релятивистской частицы со спином $s = 1/2$ (и являются интегралами движения):

а) $\hat{\mathrm{p}} = -i\hbar\nabla$

д) $\hat{\mathbf{s}}^2$

б) $\hat{\mathbf{l}} = \frac{1}{\hbar}[\hat{\mathbf{r}} \times \hat{\mathbf{p}}] = -i[\mathbf{r} \times \nabla]$

е) $\hat{\mathrm{j}} = \hat{\mathrm{i}} + \hat{\mathbf{s}}$

в) $\hat{1}^2$;

ж) $\hat{j}^2$;

г) $\hat{\mathbf{s}} = \frac{1}{\hbar}\hat{\mathbf{S}} = \frac{1}{2}\hat{\mathbf{\Sigma}}$

3) $(\hat{\mathbf{\Sigma}}\hat{\mathbf{p}})/p$

и) $\gamma^5 = -i\gamma^0\gamma^1\gamma^2\gamma^3$.

Б-2.9.2 Инвариантность уравнения Дирака

Показать, что уравнение Дирака инвариантно относительно калибровочного преобразования. Как при этом преобразуется волновая функция?

Solution

Б-2.9.3 Простейшее решение уравнения Дирака

Найти решения уравнения Дирака, описывающие свободную частицу, имеющую определенный импульс и энергию. Для конкретизации спинового состояния частицы использовать оператор $(\hat{\mathbf{\Sigma}}\mathbf{p})/p$ (продольной поляризации).

Solution

(!?!?? удивительно, все еще не отработал это!)
2.9.3. Уравнение Дирака для свободной частицы в гамильтоновой форме имеет вид

$$i\hbar\frac{\partial}{\partial t}\Psi = \hat{\mathrm{H}}_D\Psi = \left\{c(\hat{\boldsymbol{\alpha}}\hat{\mathbf{p}}) + \hat{\beta}mc^2\right\}\Psi$$

Для стационарных состояний можно записать $\Psi(\mathbf{r},t) = e^{-\frac{i}{\hbar}Et}\psi(\mathbf{r})$, причем $\psi(r)$ удовлетворяет стационарному уравнению - уравнению на собственные значения гамильтониана Дирака. Кроме того, $\psi(\mathbf{r})$ должна быть собственной функцией оператора импульса, потому что операторы трех компонент импульса $\hat{\mathbf{p}}$ коммутируют с гамильтонианом:

$$\begin{cases}\hat{\mathrm{H}}_D\psi(\mathbf{r}) = E\psi(\mathbf{r}),\\ \hat{\mathbf{p}}\psi(\mathbf{r}) = \mathbf{p}\psi(\mathbf{r}).\end{cases}$$

Условия (2) указывают на то, что решения уравнения (1) следует искать в виде плоских волн

$$\psi(\mathbf{r}) = u(\mathbf{p},E)e^{\frac{i}{\hbar}(\mathbf{pr})},$$

где $u(\mathbf{p},E)$ - не зависящий от координат и времени биспинор. Учитывая (3), перейдем к так называемой «расщепленной» форме записи стационарного уравнения Дирака:

$$\begin{cases}c(\hat{\sigma}\mathbf{p})\chi = \left(E - mc^2\right)\varphi,\\ c(\hat{\sigma}\mathbf{p})\varphi = \left(E + mc^2\right)\chi.\end{cases}$$

Здесь мы использовали формулы, выражающие дираковские матрицы в блочном виде через $\hat{\sigma}$-матрицы Паули (II.52):

$$\hat{\alpha}_i = \begin{pmatrix}0 & \hat{\sigma}_i\\ \hat{\sigma}_i & 0\end{pmatrix},\quad \hat{\beta} = \begin{pmatrix}\mathbb{1} & 0\\ 0 & -\mathbb{1}\end{pmatrix},\quad \hat{\Sigma}_i = \begin{pmatrix}\hat{\sigma}_i & 0\\ 0 & \hat{\sigma}_i\end{pmatrix},$$

а также ввели обозначения

$$u(\mathbf{p},E) = \begin{pmatrix}\varphi(\mathbf{p},E)\\ \chi(\mathbf{p},E)\end{pmatrix};\quad \varphi = \begin{pmatrix}u_1\\ u_2\end{pmatrix},\quad \chi = \begin{pmatrix}u_3\\ u_4\end{pmatrix}$$

- двухкомпонентные функции. Условие совместности системы уравнений (4) имеет вид

$$c^2(\hat{\sigma}\mathbf{p})(\hat{\sigma}\mathbf{p}) = E^2 - m^2c^4.$$

С учетом тождества $\hat{\sigma}_n\hat{\sigma}_m = \delta_{nm}\hat{1} + ie_{nmk}\hat{\sigma}_k$ (задача 2.4.13) из этого соотношения получаем

$$E = \xi E_p \equiv \xi\sqrt{c^2\mathbf{p}^2 + m^2c^4},$$

где $\xi = \pm 1 - 3$ зак энергии. Двум знакам энергии отвечают два типа решений уравнения Дирака, соответствующие различным знакам энергии в экспоненте, т. е. различным типам зависимости функций от времени. Рассмотрим далее так называемый знаковый оператор

$$\hat{\Lambda} = \frac{\hat{\mathrm{H}}_D}{\left(\hat{\mathrm{H}}_D^2\right)^{1/2}} = \frac{c(\hat{\alpha}\mathbf{p}) + \hat{\beta}mc^2}{E_\rho},$$

записанный в общем виде и в импульсном представлении. Очевидно он коммутирует с гамильтонианом $\hat{\mathrm{H}}_D$, и поэтому его собственные значения могут быть использованы для классификации состояний, собственных для $\hat{\mathrm{H}}_D$. Собственные значения оператора $\hat{\Lambda}$ есть $\xi = \pm 1$, причем $\xi = +1$ соответствует положительному ($E > 0$), а $\xi = -1$ - отрицательному знаку энергии ($E < 0$). Для свободного движения энергия E_p, импульс $\mathbf{p}$ и ξ (знак энергии) являются интегралами движения и могут одновременно принимать определенные значения. Далее, из (4) следует, что биспинор $u(\mathbf{p}, E)$ можно представить в виде

$$u(\mathbf{p}, E) = N \begin{pmatrix} \varphi \\ \frac{c(\hat{\sigma}\mathrm{p})}{\xi E_\rho + mc^2}\varphi \end{pmatrix},$$

где N - нормировочный коэффициент, а φ - остающийся пока неопределенным двухкомпонентный спинор, нормируемый условием $\varphi^+\varphi = 1$. Нормировочный коэффициент в (8) легко находится:

$$N = \frac{1}{\sqrt{2}}\sqrt{1 + \xi\frac{mc^2}{E_p}}.$$

Осталось найти функцию φ. Неоднозначность в выборе φ связана с наличием спиновой степени свободы у дираковской частицы, Рассмотрим оператор $(\hat{\Sigma}\mathbf{p})/p$, где $p = |\mathbf{p}|$. Собственные значения этого оператора характеризуют проекцию спина на направление движения, т. е. это оператор продольной поляризации. Оператор продольной поляризации коммутирует с гамильтонианом, следовательно, физическая величина, соответствующая ему, является интегралом движения. Поэтому к уравнениям (2) можно добавить уравнение

$$\frac{(\hat{\mathbf{\Sigma}}\mathbf{p})}{p}\psi(\mathbf{r}) = s\psi(\mathbf{r})$$

где собственное значение $s = \pm 1$ называется спиральностью частицы. Используя (8), а также явный вид матриц $\hat{\Sigma}_i$(5), сводим это уравнение к двухкомпонентному:

$$(\hat{\sigma}\mathrm{p})\varphi = sp\varphi,$$

т. е. к уравнению для паулиевских спиноров с определенным значением проекции спина на направление импульса. Ясно, что уравнение (9) определяет двухкомпонентный спинор, собственный для оператора $(\hat{\sigma}\mathbf{n})$, где $\mathbf{n} = \mathbf{p}/p$. Такие функции были найдены нами в задаче 2.4.19. На этом можно было бы и завершить решение данной задачи, но представ- ляется полезным получить также другой вид решения уравнения (9) с явной зависимостью от спиральности s. Такое решение может быть представлено в виде

$$\varphi_s = \frac{1}{\sqrt{2}}\begin{pmatrix} (1 + sp_z/p)^{1/2} \\ s\,(1 - sp_z/p)^{1/2}\,e^{i\delta} \end{pmatrix}.$$

где $\mathrm{tg}\,\delta = p_y/p_x$. Если ввести сферические координаты вектора $\mathbf{n} = \mathbf{p}/p$, то эти функции перейдут в функции $\Psi_{\pm!}$задачи 2.4.19. Объединяя наши результаты (10) и (8), мы получаем нормированные собственные функции операторов $\hat{\mathrm{H}}_D, \hat{\mathbf{p}}, \hat{\Lambda}$ и $(\hat{\mathbf{\Sigma}}\mathbf{p})/p$:

$$\Psi_{\mathrm{p},\xi,s}(\mathbf{r}, t) = \frac{e^{-\frac{i}{\hbar}(\xi E_p - pr)}}{2\sqrt{V}}\begin{pmatrix} \left(1 + \xi\frac{mc^2}{E_p}\right)^{1/2}\left(1 + s\frac{p_z}{p}\right)^{1/2} \\ s\left(1 + \xi\frac{mc^2}{E_p}\right)^{1/2}\left(1 - s\frac{p_z}{p}\right)^{1/2}e^{i\delta} \\ s\xi\left(1 - \xi\frac{mc^2}{E_p}\right)^{1/2}\left(1 + s\frac{p_z}{p}\right)^{1/2} \\ \xi\left(1 - \xi\frac{mc^2}{E_p}\right)^{1/2}\left(1 - s\frac{p_z}{p}\right)^{1/2}e^{i\delta} \end{pmatrix}.$$

Б-2.9.4 Скорость дираковской частицы (!?!??!?)

а) Найти оператор скорости $\hat{\mathrm{v}}_x$ в теории Дирака в случае свободного движения.
б) Показать, что четная часть этого оператора $[\hat{\mathrm{v}}_x]$ допускает простую классическую интерпретацию.
в) Показать, что его нечетная часть $\{\hat{\mathrm{v}}_x\}$ осциллирует с частотой $\omega = 2E/\hbar$ (Zitterbewegung).

Указание: оператор, описывающий физическую величину $\hat{\mathrm{F}}$, можно записать в виде $\hat{F} = [\hat{F}] + \{\hat{F}\}$, где

$$[\hat{\mathrm{F}}] = \frac{1}{2}(\hat{\mathrm{F}} + \hat{\Lambda}\hat{\mathrm{F}}\hat{\Lambda}), \quad \{\hat{\mathrm{F}}\} = \frac{1}{2}(\hat{\mathrm{F}} - \hat{\Lambda}\hat{\mathrm{F}}\hat{\Lambda}); \quad \hat{\Lambda} = \frac{\hat{\mathrm{H}}}{E}.$$

Solution

2.9.4. Перейдем в гейзенберговское представление и вычислим оператор $d\hat{x}/dt$, представляющий собой, очевидно, x-компоненту оператора скорости:

$$\frac{d\hat{x}}{dt} = \hat{\mathrm{v}}_x = \frac{i}{\hbar}\left[\hat{\mathrm{H}}_D, \hat{x}\right] = \frac{i}{\hbar} c\hat{\alpha}_1 \left[\hat{\mathrm{p}}_x, \hat{x}\right] = c\hat{\alpha}_1.$$

Данный результат не поддается интерпретации в духе принципа соответствия. Во-первых, поскольку собственные значения оператора $\hat{\alpha}_1$ равны ± 1, то оказывается, что собственные значения операторов компонент скорости равны $\pm c$, хотя в действительности скорость может принимать любые значения в промежутке от $-c$ до $+c$. Во-вторых, матрицы $\hat{\alpha}_i$ не коммутируют между собой, что должно приводить к принципиальной невозможности одновременно измерить хотя бы две компоненты скорости.

И, наконец, в теории Дирака происходит так называемое «расщепление» понятий скорости и импульса, т. е. отсутствуют обычные, аналогичные существующим в релятивистской классической механике связи между операторами скорости и импульса. Эти сложности в физической интерпретации оператора скорости, связаны с интерференцией состояний с различными знаками энергии.

В последовательной одночастичной теории физические величины должны описываться операторами, не смешивающими между собой состояния с различными знаками энергии. Такие операторы называются четными (или «одночастичными»). Четный оператор переводит волновую функцию с определенным знаком энергии в функцию с тем же знаком энергии, а нечетный оператор - в функцию с другим знаком энергии:

$$[\hat{\mathrm{F}}]\Psi(\pm) = \widetilde{\Psi}(\pm), \quad \{\hat{\mathrm{F}}\}\Psi(\pm) = \widetilde{\Psi}(\mp).$$

Найдем четную часть оператора скорости:

$$[\hat{\mathrm{v}}_x] = c\,[\hat{\alpha}_1] = \frac{1}{2}\left(\hat{\mathrm{v}}_x + \hat{\Lambda}_x\hat{\mathrm{v}}_x\right) = \frac{c}{2E_\rho}\left\{\hat{\alpha}_1, \hat{\mathrm{H}}_D\right\}\hat{\Lambda} = \frac{c^2 p_x}{E_\rho}\hat{\Lambda}.$$

Отсюда следует, что четная часть оператора скорости для решений с положительной энергией ($\xi = +1$) связана с оператором импульса соотношением, соответствующим связи между скоростью и импульсом в классической релятивистской теории - четная часть оператора скорости допускает простую классическую интерпретацию.

Нечетная часть оператора скорости $\{\hat{\mathrm{v}}_x\} = \frac{1}{2}\left(\hat{\mathrm{v}}_x - \hat{\Lambda}\hat{\mathrm{v}}_x\hat{\Lambda}\right)$ антикоммутирует с гамильтонианом, потому что

$$\frac{\hat{\mathrm{H}}_D}{E_\rho}\{\hat{\mathrm{v}}_x\} = \frac{1}{2}\left(\hat{\Lambda}\hat{\mathrm{v}}_x - \hat{\mathrm{v}}_x\hat{\Lambda}\right) = -\{\hat{\mathrm{v}}_x\}\frac{\hat{\mathrm{H}}_D}{E_\rho}.$$

Отсюда следует, что

$$\frac{d}{dt}\{\hat{\mathrm{v}}_x\} = \frac{i}{\hbar}\left[\hat{\mathrm{H}}_D, \{\hat{\mathrm{v}}_x\}\right] = -\frac{2i}{\hbar}\{\hat{\mathrm{v}}_x\}\hat{\mathrm{H}}_D.$$

Интегрирование этого уравнения с учетом $\partial\hat{\mathrm{H}}_D/\partial t = 0$ дает

$$\{\hat{\mathrm{v}}_x\} = c\{\hat{\alpha}_1\} = c\{\hat{\alpha}_1(0)\}\, e^{-\frac{2i\hat{\mathrm{H}}_D t}{\hbar}}.$$

Таким образом, нечетная часть оператора скорости не имеет классического аналога и характеризуется быстрыми осцилляциями с частотой $\sim 2|E|/\hbar$, вызывая явление Zitterbewegung («дрожащее движение»), которое, по существу, и затрудняет физическую интерпретацию операторов в теории Дирака.

Б-2.9.5 Парадокс Клейна: рождение пары частиц в поле

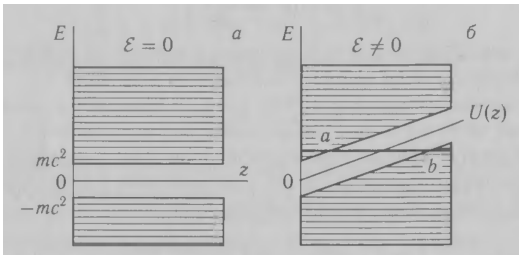
Оценить вероятность рождения пары e^+e^--пары в однородном постоянном электрическом поле в квазиклассическом приближении (парадокс Клейна).

Solution

2.9.5. Система уровней энергии свободного электрона Дирака

$$E = \xi\sqrt{c^2\mathbf{p}^2 + m^2c^4}, \quad \xi = \pm 1$$

представляет собой два континуума состояний для положительных и отрицательных значений энергии, которые разделены энергетической щелью $\Delta E = 2mc^2$ (рис. 2.11, a).



Предположим, что электрон находится в постоянном и однородном электрическом поле, направленном вдоль оси z. Пусть движ ение происходит вдоль поля $\mathcal{E}=\{0,0,\mathcal{E}\}$.

При этом существенно изменяется конфигурация уровней энергии электрона: изменяются границы верхнего $\left(E=mc^2\right)$ и нижнего $\left(E=-mc^2\right)$ континуумов энергии (рис. 2.11, 6).

Новыми границами верхнего и нижнего континуумов состояний станут линии

$$E=\pm mc^2+e\mathcal{E}z,$$

где $U(z)=e\varepsilon z$ - потенциальная энергия электрона в электрическом поле (подразумевается $-e<0$ - заряд электрона). В результате поворота запрещенной энергетической зоны, разделяющей верхний и нижний континуумы, состояния с отрицательной и положительной энергией будут разделены лишь пространственно.

Таким образом, электрон, имеющий определенную энергию E, будет находиться в есостоянии с положительной энергией ($\xi=+1$) при $z\leqslant a$ и в есостоянии с отрицательной энергией ($\xi=-1$) при $z\geqslant b$. Но на самом деле (рис. 2.11) энергия электрона при этом остается одной и той же. Значит, при наличии внешнего электрического поля (или любого другого потенциала) не может быть строгого разделения состояний на состояния с положительной и отрицательной энергией. Более того, возможен туннельный переход через запрещенную зону из верхнего континуума в нижний (или наоборот). Этот эффект и представляет собой парадокс Клейна.

Оценим вероятность туннельного перехода из верхнего континуума в нижний, используя квазиклассическое приближение (II.38):

$$D\simeq\exp\left\{-\frac{2}{\hbar}\int\limits_a^b|p(z)|dz\right\}.$$

где $|p(z)|=\frac{1}{c}\sqrt{m^2c^4-(E-e\mathcal{E}z)^2}$. Вычисляем интеграл и получаем, что

$$D\simeq\exp\left\{-\pi\frac{m^2c^3}{e\hbar\mathcal{E}}\right\}.$$

Очевидно, что такой же вид должна иметь и вероятность обратного туннельного перехода - из нижнего континуума в верхний.

Итак, наложение электрического поля не приводит к локализации дираковской частицы - она может оказаться в состоянии с противоположным знаком энергии в результате туннельного перехода, причем вероятность такого перехода растет с ростом поля и стремится к единице в том случае, если напряженность поля равна

$$\mathcal{E}=\mathcal{E}_{\text{кр}}=\frac{m^2c^3}{e\hbar}=1,3\cdot10^{16}\text{ В/см}$$

- так называемому швингеровскому значению. В соответствии с дырочной интерпретацией Дирака при переходе электрона из нижнего континуума состояний в верхний появляется пара частиц: электрон в верхнем континууме с энергией $E>0$ и едырка в нижнем континууме (среди состояний с $E<0$). Эта едырка» интерпретируется, как античастица по отношению к электрону, т.е. позитрон. Следовательно, мы описали процесс рождения электрон-позитронной пары.

Б-2.9.6 нерелятивистский предел уравнения Дирака

Показать, что в нерелятивистском пределе уравнение Дирака переходит в уравнение Паули.
(мб удалю и просто в теории будет это, чисто типичная теория)

Solution

2.9.6. Уравнение Дирака, описывающее движение заряженной частицы во внешнем электромагнитном поле, имеет вид

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t)=\left(c(\hat{\alpha}\hat{\mathcal{P}})+\hat{\beta}mc^2-e\phi\right)\Psi(\mathbf{r},t).$$

где $\hat{\mathcal{P}} = \hat{\mathbf{p}} + \frac{e}{c}\mathbf{A}$, $-e < 0$ - заряд электрона. Считаем состояние $\Psi(\mathbf{r}, t)$ стационарным: $\Psi(\mathbf{r}, t) = e^{-\frac{i}{\hbar}Et}\psi(\mathbf{r})$. В дальнейшем будем полагать $E > 0$, т. е. мы фиксируем знак энергии (считаем энергию положительной, ибо в нерелятивистской квантовой механике имеются только состояния с положительной энергией). Представим далее, как и обычно, волновую функцию в виде $\psi(\mathbf{r}) = \begin{pmatrix} \varphi(\mathbf{r}) \\ \chi(\mathbf{r}) \end{pmatrix}$ и запишем (1) в «расщепленномь виде:

$$\begin{cases} \left(E - mc^2 + e\phi\right)\varphi = c(\hat{\sigma}\hat{\mathcal{P}})\chi. \\ \left(E + mc^2 + e\phi\right)\chi = c(\hat{\sigma}\hat{\mathcal{P}})\varphi. \end{cases}$$

Исследуем эту систему в нерелятивистском пределе и в слабых полях, т. е.

$$E \simeq mc^2 + \varepsilon, \quad |\varepsilon + e\phi| \ll mc^2.$$

В этом случае (2) перейдет в

$$\begin{cases} (\varepsilon + e\phi)\varphi(\mathbf{r}) = c(\hat{\boldsymbol{\sigma}}\hat{\mathcal{P}})\chi(\mathbf{r}) \\ \left(\varepsilon + e\phi + 2mc^2\right)\chi(\mathbf{r}) = c(\hat{\boldsymbol{\sigma}}\hat{\mathcal{P}})\varphi(\mathbf{r}) \end{cases}$$

Из второго уравнения с учетом (3) находим

$$\gamma(\mathbf{r}) \simeq \frac{(\hat{\sigma}\hat{\mathcal{P}})}{2mc}\varphi(\mathbf{r}),$$

откуда видно, что в нерелятивистском приближении двухкомпонентный спинор $\chi(\mathbf{r})$ имеет по отношению к $\varphi(\mathbf{r})$ порядок малости $(v/c) \ll 1$. Это и позволяет (в случае положительной энергии $E > 0$) говорить о двух нижних компонентах дираковского спинора как о малых.

Подставим (4) в первое уравнение системы и получим с линейной точностью по (v/c) уравнение для двухкомпонентного спинора $\varphi(\mathbf{r})$:

$$(\varepsilon + e\phi)\varphi(\mathbf{r}) = \frac{1}{2m}(\hat{\sigma}\hat{\mathcal{P}})(\hat{\boldsymbol{\sigma}}\hat{\mathcal{P}})\varphi(\mathbf{r}).$$

Преобразуя правую часть данного уравнения, находим

$$\begin{aligned}(\hat{\sigma}\hat{\mathcal{P}})(\hat{\sigma}\hat{\mathcal{P}}) = \hat{\mathcal{P}}_i\hat{\mathcal{P}}_i\left(\delta_{ij} + ie_{ijk}\hat{\sigma}_k\right) =& \hat{\mathcal{P}}^2 + i\frac{e}{c}\hat{\sigma}_k e_{ijk}\left(\hat{p}_i\ \mathrm{A}_i + \mathrm{A}_i\hat{\mathrm{p}}_j\right) = \\ &= \hat{\mathcal{P}}^2 + i\frac{e}{c}\hat{\sigma}_k e_{i/k}\left[\hat{p}_i,\ \mathrm{A}_j\right] = \hat{\mathcal{P}}^2 + \frac{e\hbar}{c}(\hat{\sigma}\mathcal{H}),\end{aligned}$$

где $\mathcal{H} = \operatorname{rot}\mathbf{A}$. В результате получаем нерелятивистское уравнение, описывающее движение частицы со спином $1/2$ в электромагнитном поле:

$$\left(\frac{\hat{\mathcal{P}}^2}{2m} + \frac{eh}{2mc}(\hat{\sigma}\mathcal{H}) - e\phi\right)\varphi(\mathbf{r}) = \varepsilon\varphi(\mathbf{r}).$$

Это и есть уравнение Паули, а $\varphi(\mathbf{r})$ - паулиевский двухкомпонентный спинор.

Б-2.9.7

Найти релятивистские поправки порядка $(v/c)^2$ к нерелятивистскому гамильтониану атома водорода с помощью разложения гамильтониана Дирака, описывающего состояния в кулоновском поле ядра, по степеням v/c. Провести классификацию полученных поправок.

Solution

2.9.7. В уравнении Дирака для электрона во внешнем электромагнитном поле

$$ih\frac{\partial}{\partial t}\Psi(\mathbf{r}, t) = \left(c(\hat{\alpha}\hat{\mathcal{P}}) + \hat{\beta}mc^2 - e\phi\right)\Psi(\mathbf{r}, t)$$

положим

$$U(r) = -e\phi(r) = -\frac{Ze^2}{r}, \quad \mathbf{A} = 0,$$

т. е. будем считать, что внешнее поле - чисто кулоновское, при этом, очевидно, $\hat{\mathcal{P}} = \hat{\mathbf{p}} + \frac{e}{c}\mathbf{A} \to \hat{\mathbf{p}}$, и, как и ранее, $-e < 0$ - заряд электрона.

Полагаем, что задача - стационарная: $\Psi(\mathbf{r}, t) = e^{-\frac{i}{\hbar}Et}\psi(\mathbf{r})$, фиксируем знак энергии $E > 0$. Переходим к «расщепленной форме записи уравнения Дирака:

$$\psi(\mathbf{r}) = \begin{pmatrix} \varphi(\mathbf{r}) \\ \chi(\mathbf{r}) \end{pmatrix}; \begin{cases} \left(E - mc^2 + e\phi\right)\varphi = c(\hat{\sigma}\hat{\mathbf{p}})\chi, \\ \left(E + mc^2 + e\phi\right)\chi = c(\hat{\boldsymbol{\sigma}}\hat{\mathbf{p}})\varphi. \end{cases}$$

Из второго уравнения системы (1) выражаем $\chi(\mathbf{r})$:

$$\chi(\mathbf{r}) = \frac{1}{E + mc^2 + e\phi} c(\hat{\sigma}\hat{\mathbf{p}})\varphi(\mathbf{r})\Big|_{\frac{e}{c}\to 0} \simeq \frac{(\hat{\sigma}\hat{\mathbf{p}})}{2mc^2}\varphi(\mathbf{r}).$$

т. е. в нерелятивистском приближении функция $\chi(\mathbf{r})$ имеет по отношению к $\varphi(\mathbf{r})$ порядок малости $(v/c) \ll 1$. Подставляем результат (2) в первое уравнение (1) и получим (пока еще точное) уравнение для $\varphi(\mathbf{r})$:

$$\left(E - mc^2 + e\phi\right)\varphi(\mathbf{r}) = c^2(\hat{\sigma}\hat{\mathbf{p}})\frac{1}{E + mc^2 + e\phi}(\hat{\sigma}\hat{\mathbf{p}})\varphi(\mathbf{r}).$$

Переходим к нерелятивистскому приближению:

$$E \simeq mc^2 + \varepsilon, \quad |\varepsilon + e\phi| \ll mc^2.$$

и в дальнейшем при разложениях будем ограничиваться членами порядка $(v/c)^2$. Поэтому

$$\left(E + mc^2 + e\phi\right)^{-1} = \left(2mc^2 + \varepsilon + e\phi\right)^{-1} \simeq \frac{1}{2mc^2}\left(1 - \frac{\varepsilon + e\phi}{2mc^2}\right).$$

При этом уравнение (3) принимает вид

$$\left(\varepsilon + e\phi - \frac{\hat{\mathbf{p}}^2}{2m}\right)\varphi(\mathbf{r}) = -(\hat{\sigma}\hat{\mathbf{p}})\frac{\varepsilon + e\phi}{4m^2c^2}(\hat{\sigma}\hat{\mathbf{p}})\varphi(\mathbf{r}).$$

В правой части уравнения (4) преобразуем слагаемое

$$\begin{aligned} -(\hat{\sigma}\hat{\mathbf{p}})e\phi(\hat{\sigma}\hat{\mathbf{p}}) = (\hat{\sigma}\hat{\mathbf{p}})U(r)(\hat{\sigma}\hat{\mathbf{p}}) = U(r)\hat{\mathbf{p}}^2 + [(\hat{\sigma}\hat{\mathbf{p}}), U(r)](\hat{\sigma}\hat{\mathbf{p}}) = \\ = U(r)\hat{\mathbf{p}}^2 + \left(\delta_{ij} + ie_{ijk}\hat{\sigma}_k\right)\left(-i\hbar\nabla_i U(r)\right)\hat{\mathrm{p}}_i = \\ = U(r)\hat{\mathbf{p}}^2 - ih((\nabla U(r))\hat{\mathbf{p}}) + \hbar^2\frac{dU(r)}{dr}\frac{1}{r}(\hat{\boldsymbol{q}}\hat{l}). \end{aligned}$$

Здесь $\hat{\mathbf{l}} = \frac{1}{\hbar}[\hat{\mathbf{r}} \times \hat{\mathbf{p}}]$ - орбитальный момент. Уравнение (4) при этом перейдет в

$$\begin{aligned} \left(\varepsilon + e\phi - \frac{\hat{\mathbf{p}}^2}{2m}\right)\varphi(\mathbf{r}) = \\ = \left\{-\frac{\varepsilon + e\phi}{4m^2c^2}\hat{\mathbf{p}}^2 + \frac{\hbar}{4m^2c^2}\left[-i((\nabla U(r))\hat{\mathbf{p}}) + \hbar\frac{dU(r)}{dr}\frac{(\sigma\mathrm{i})}{r}\right]\right\}\varphi(\mathbf{r}). \end{aligned}$$

Далее, в правой части (6) преобразуем первое слагаемое:

$$\begin{aligned} (\varepsilon + e\phi)\hat{\mathbf{p}}^2 = \hat{\mathbf{p}}^2(\varepsilon + e\phi) + \left[(\varepsilon + e\phi), \hat{\mathbf{p}}^2\right] \simeq \frac{\hat{\mathbf{p}}^4}{2m} - \hat{\mathbf{p}}|U(r), \hat{\mathbf{p}}| - |U(r), \hat{\mathbf{p}}|\hat{\mathbf{p}} = \\ = \frac{\hat{\mathbf{p}}^4}{2m} - \hbar^2\left(\nabla^2 U(r)\right) - 2i\hbar((\nabla U(r))\hat{\mathbf{p}}). \end{aligned}$$

Здесь мы учли, что на решениях уравнения в рассматриваемом приближении $(\varepsilon + e\phi)\varphi(\mathbf{r}) \simeq \frac{\hat{\mathbf{p}}^2}{2m}\varphi(\mathbf{r})$, а также использовали правило дифференцирования произведения функций.

Теперь вспомним общий вид нашей (четырехкомпонентной) волновой функции (1) с учетом (2). Запишем условие нормировки функции $\psi(\mathbf{r})$ с точностью до $(v/c)^2$:

$$\mathrm{I} = \int \psi^+(\mathbf{r})\psi(\mathbf{r})d^3x \simeq \int d^3x\left\{\varphi^+(\mathbf{r})\varphi(\mathbf{r}) + \frac{\hbar^2}{4m^2c^2}((\hat{\boldsymbol{\sigma}}\nabla)\varphi(\mathbf{r}))^+((\hat{\boldsymbol{\sigma}}\nabla)\varphi(\mathbf{r}))\right\}.$$

Здесь мы использовали вид оператора импульса: $\hat{\mathbf{p}} = -i\hbar\boldsymbol{\nabla}$. Заметим, что мы хотим получить приближенное уравнение для двухкомпонентной паулиевской (нерелятивистской) функции, которую в дальнейшем будем обозначать $\psi^{\Pi}(\mathbf{r})$. Две компоненты такой функции должны, как всегда, описывать две возможные ориентации спина, и условие нормировки для $\psi^{\Pi}(\mathbf{r})$ должно иметь традиционный вид:

$$1 = \int \psi^{\Pi+}(\mathbf{r})\psi^{\Pi}(\mathbf{r})d^3x.$$

Наше приближенное уравнение (6) пока записано для двухкомпонентной функцин $\varphi(\mathbf{r})$ (верхние компоненты биспинора $\psi(\mathbf{r})$), но функция $\varphi(\mathbf{r})$ имеет существенно иное условие нормировки, следующее из (8).

В связи с этим в условии нормировки (8) проинтегрируем по частям второе слагаемое:

$$\int d^3x((\hat{\sigma}\nabla)\varphi)^+((\hat{\sigma}\nabla)\varphi) = -\int d^3x\varphi^+(\Delta\varphi) = -\int d^3x\left(\Delta\varphi^+\right)\varphi.$$

Симметризуя эти два варианта, из условия (8) мы получим

$$1 = \int d^3x\left\{\varphi^+\varphi - \frac{\hbar^2}{8m^2c^2}\left[\left(\Delta\varphi^+\right)\varphi + \varphi^+(\Delta\varphi)\right]\right\}.$$

Для согласования нормировочных условий (9) и (10) с точностью до $(v/c)^2$ положим

$$\psi^{\Pi}(\mathbf{r}) = \left(1 + \frac{\hat{\mathbf{p}}^2}{8m^2c^2}\right)\varphi(\mathbf{r}), \quad \text{или } \varphi(\mathbf{r}) = \left(1 - \frac{\hat{\mathbf{p}}^2}{8m^2c^2}\right)\psi^{\Pi}(\mathbf{r}),$$

где мы учли, что $\hat{\mathbf{p}}^2 = -\hbar^2\Delta$. Это есть не что иное, как каноническое преобразование волновой функции, ибо оно сохраняет значение нормировочного интеграла, т. е. вероятность.

Теперь подставим в уравнение (6) соотношение (7), а также функцию $\varphi(\mathbf{r})$, выраженную через $\psi^{\Pi}(\mathbf{r})$. В итоге получим окончательный вид приближенного уравнения:

$$\left(\varepsilon + e\phi - \frac{\hat{\mathbf{p}}^2}{2m}\right)\psi^{\Pi}(\mathbf{r}) = \hat{\mathrm{V}}\psi^{\Pi}(\mathbf{r})$$

$$\hat{\mathrm{V}} = -\frac{\hat{\mathbf{p}}^4}{8m^3c^2} + \frac{\hbar^2}{2m^2c^2}\frac{dU}{dr}\frac{(\hat{\mathbf{s}}\hat{i})}{r} + \frac{1}{8}\left(\frac{\hbar}{mc}\right)^2\left(\nabla^2 U\right).$$

В правой части полученного уравнения сгруппированы поправки к движению электрона в кулоновском поле. В порядке следования это: релятивистская поправка, спин-орбитальное взаимодействие и контактное взаимодействие.

Б-2.9.8

Найти энергетический спектр заряженной дираковской частицы в однородном магнитном поле.

Solution

2.9.8. Пусть магнитное поле направлено по оси $z : \mathcal{H} = \{0, 0, \mathcal{H}\}$. Выберем вектор-потенциал так же, как в нерелятивистском случае в задаче 2.5.1, т. е. $\mathbf{A} = \{0, \mathcal{H}x, 0\}$. Тогда стационарное уравнение Дирака будет иметь вид $\hat{\mathrm{H}}_D\psi(\mathbf{r}) = E\psi(\mathbf{r})$, причем

$$\hat{\mathrm{H}}_D = c(\hat{\boldsymbol{\alpha}}\hat{\mathcal{P}}) + \hat{\beta}mc^2, \quad \hat{\mathcal{P}} = \hat{\mathbf{p}} + \frac{e}{c}\mathbf{A}, \quad -e < 0$$

- заряд электрона. Перейдем к «расщепленной» форме записи уравнения Дирака:

$$\psi(\mathbf{r}) = \begin{pmatrix} \varphi(\mathbf{r}) \\ \chi(\mathbf{r}) \end{pmatrix}; \begin{cases} c(\hat{\boldsymbol{\sigma}}\hat{\mathcal{P}})\chi = \left(E - mc^2\right)\varphi, \\ c(\hat{\boldsymbol{\sigma}}\hat{\mathcal{P}})\varphi = \left(E + mc^2\right)\chi. \end{cases}$$

Выразим из второго уравнения системы (1) $\chi(\mathbf{r})$ через $\varphi(\mathbf{r})$ и подставим результат в первое уравнение:

$$\left(E^2 - m^2c^4\right)\varphi(\mathbf{r}) = c^2(\hat{\boldsymbol{\sigma}}\hat{\mathcal{P}})(\hat{\boldsymbol{\sigma}}\hat{\mathcal{P}})\varphi(\mathbf{r}).$$

Используем тождество (задача 2.9.6) $(\hat{\sigma}\hat{\mathcal{P}})(\hat{\sigma}\hat{\mathcal{P}}) = \hat{\mathcal{P}}^2 + \frac{e\hbar}{c}(\hat{\sigma}\mathcal{H})$, и тогда уравнение (2) примет вид

$$\left\{\hat{\mathrm{p}}_x^2 + \left(\hat{\mathrm{p}}_y + \frac{e}{c}\mathcal{H}x\right)^2 + \hat{\mathrm{p}}_z^2 + \frac{e\hbar}{c}\mathcal{H}\hat{\sigma}_z\right\}\varphi(\mathbf{r}) = \frac{E^2 - m^2c^4}{c^2}\varphi(\mathbf{r}).$$

Полученное уравнение формально имеет вид уравнения Шредингера $\hat{\mathrm{H}}_{\text{eff}}\varphi(\mathbf{r}) = E_{\text{eff}}\,\varphi(\mathbf{r})$, причем легко заметить, что $\hat{\mathrm{H}}_{\text{eff}}$ коммутирует с операторами $\hat{\mathrm{p}}_y$ и $\hat{\mathrm{p}}_z$. Это значит, что можно искать решение уравнения (3) в виде

$$\varphi(\mathbf{r}) = Ce^{\frac{i}{\hbar}(p_y y + p_z z)}f(x).$$

Далее положим $f(x) = \begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix}$ и приведем уравнение (3) к следующему виду:

$$\left\{\frac{\hat{p}_x^2}{2m} + \frac{m}{2}\left(\frac{e\mathcal{H}}{mc}\right)^2\left(x + \frac{cp_y}{e\mathcal{H}}\right)^2\right\}f_{1,2}(x) = \frac{1}{2mc^2}\left[E^2 - m^2c^4 \mp e\hbar c\mathcal{H} - c^2p_z^2\right]f_{1,2}(x).$$

Уравнение (5) есть не что иное, как нерелятивистское уравнение для осциллятора $\hat{\mathrm{H}}'_{\text{eff}}f_{1,2}(x) = E'_{\text{eff}}\,f_{1,2}(x)$, причем

$$\hat{\mathrm{H}}'_{\text{eff}} = \frac{\hat{\mathrm{p}}_x^2}{2m} + \frac{m}{2}\Omega^2x'^2, \quad x' = x + \frac{cp_y}{e\mathcal{H}}, \quad \Omega = \frac{e\mathscr{H}}{mc}, \quad \frac{d^2}{dx^2} = \frac{d^2}{dx'^2}.$$

Ясно, что должно выполняться $E'_{\text{eff}} = \hbar\Omega\,(n' + 1/2)$ и на основании этого получаем

$$E^2 - m^2c^4 - c^2p_z^2 = e\hbar c\mathcal{H}\,(2n' + 1 \pm 1)\,.$$

Очевидно, что $2n' + 1 \pm 1$ - всегда четное число. Обозначим его $2n$ и получим окончательный результат:

$$E_{np_z} = \sqrt{m^2c^4 + c^2p_z^2 + 2e\hbar c\mathcal{H}n}.$$

Поскольку в соотношении $2n' + 1 \pm 1 = 2n$ знак $\pm$ относится к компонентам $f_{1,2}(x)$ функции $f(x)$, то ясно, что общий вид функции $\varphi(\mathbf{r})$ (формула (4)) должен быть таким:

$$\varphi_{\pi p_y p_z}(\mathbf{r}) = \exp\left[\frac{i}{\hbar}\,(p_y y + p_z z)\right]\begin{pmatrix} C_1 u_{n-1}^{\text{oclu}}\,(x') \\ C_2 u_n^{\text{ocll}}\,(x') \end{pmatrix}.$$

где $u_n^{\text{ocu}}\,(x)$ есть обычное решение уравнения Шредингера для гармонического осциллятора (II.18). Коэффициенты $C_{1,2}$ можно определить, если конкретизировать спиновое состояние частицы, для этого нужен еще один оператор - спиновый интеграл движения.

Найденные нами уровни энергии (6) не являются эквидистантными в отличие от уровней Ландау (задача 2.5.1). Уровни энергии вырождены по спину с кратностью 2 (кроме основного состояния $n = 0$) и по p_y - с бесконечной кратностью.

Б-2.9.9

Найти в нерелятивистском пределе выражение для плотности заряда и тока заряженной дираковской частицы, находящейся во внешнем электромагнитном поле.

Solution

Б-2.9.10

Показать, что преобразование зарядового сопряжения позволяет интерпретировать решения уравнения Дирака с отрицательными значениями энергии как волновые функции античастиц.

Solution

2.9.11. Мы полагаем, что нейтрино - нейтральные массивные дираковские частицы. Кроме того, мы считаем, что нейтрино определенного типа (например, электронное или мюонное), или, как принято говорить, определенного аромата, не являются состояниями с определенной массой, а представляют собой суперпозицию таких состояний:

$$\begin{cases} |\nu_e\rangle = |\nu_1\rangle\cos\theta + |\nu_2\rangle\sin\theta, \\ |\nu_\mu\rangle = -|\nu_1\rangle\sin\theta + |\nu_2\rangle\cos\theta. \end{cases}$$

Состояния $|\nu_{1,2}\rangle$ в (1) удовлетворяют уравнениям Дирака соответственно с массами m_1 и m_2, а θ - угол смешивания нейтрино. Эволюция во времени состояний $|\nu_1\rangle$ и $|\nu_2\rangle$ дается выражением

$$|\nu_1(t)\rangle = e^{-\frac{i}{\hbar}E_1 t}|\nu_1(0)\rangle; \quad |\nu_2(t)\rangle = e^{-\frac{i}{\hbar}E_2 t}|\nu_2(0)\rangle.$$

где $E_{1,2} = \sqrt{\mathbf{p}^2c^2 + m_{1,2}^2c^4}$. Если в момент $t = 0$ рождается электронное нейтрино, то его состояние эволюционирует во времени следующим образом:

$$\begin{aligned}|\nu_e(t)\rangle &= \cos\theta e^{-\frac{i}{\hbar}E_1 t}|\nu_1(0)\rangle + \sin\theta e^{-\frac{i}{\hbar}E_2 t}|\nu_2(0)\rangle = \\ &= \left(e^{-\frac{i}{\hbar}E_1 t}\cos^2\theta + e^{-\frac{i}{\hbar}E_2 t}\sin^2\theta\right)|\nu_e(0)\rangle + \\ &+ \cos\theta\sin\theta\left(e^{-\frac{i}{\hbar}E_2 t} - e^{-\frac{i}{\hbar}E_1 t}\right)|\nu_\mu(0)\rangle.\end{aligned}$$

Вероятность того, что нейтрино, родившись в момент $t = 0$, как электронное, перейдет в момент t в состояние $|\nu_\mu\rangle$, имеет вид

$$P(\nu_e \to \nu_\mu) = |\langle\nu_\mu|\nu_e(t)\rangle|^2 = \frac{1}{2}\sin^2 2\theta\left[1 - \cos\frac{\left(m_2^2 - m_1^2\right)c^3}{2p\hbar}t\right].$$

Здесь мы предположили, что $p \gg m_{1,2}c$. Вероятность появления нейтрино нового сорта периодически зависит от времени, поэтому яанное явление и носит название осцилляций.

Описание столкновения двух электронов с помощью уравнения Дирака (??)

(??? завис вопрос, хз, что сделать, как решат такое? пока супер слабая теория для этого.)

Б-2.9.11 осцилляции нейтрино (??)

Предполагая, что состояния электронного и мюонного нейтрино представляют собой суперпозиции состояний нейтрино $|\nu_1\rangle$ и $|\nu_2\rangle$ с определенными массами m_1 и m_2:

$$\begin{cases} |\nu_e\rangle = |\nu_1\rangle\cos\theta + |\nu_2\rangle\sin\theta, \\ |\nu_\mu\rangle = -|\nu_1\rangle\sin\theta + |\nu_2\rangle\cos\theta, \end{cases}$$

найти вероятность перехода нейтрино в состояние $|\nu_\mu\rangle$ к моменту времени t, если при $t = 0$ оно было электронным (осцилляции нейтрино).

(в 1ю часть продублирую мб)

20.5.2 Problems about the Heisenberg Formalism (??)

(пока не знаю отдельные такие, пусть повесит раздел, мб удалю.)

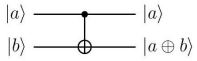
20.6 Problems on the Foundations of Quantum Information Theory

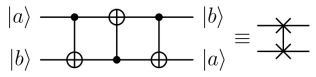
(тут прорешаю еще раз Филиппова, если что на сайте кафедры многие его задачи, так что в них разберусь. подробнее - в записи по квантовой теории информации. не такое тривиальное тут!)

(see note on quantum information about it for now)

20.6.1 Problems on basic quantum gates

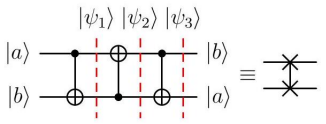
KUL-2023-10.1.1 Quantum circuits

Consider the CNOT gate 

where $\oplus$ is the addition modulo 2. Show that the SWAP gate 

is indeed swapping the state of the two qubits, i.e. $|a, b\rangle \to |b, a\rangle$.

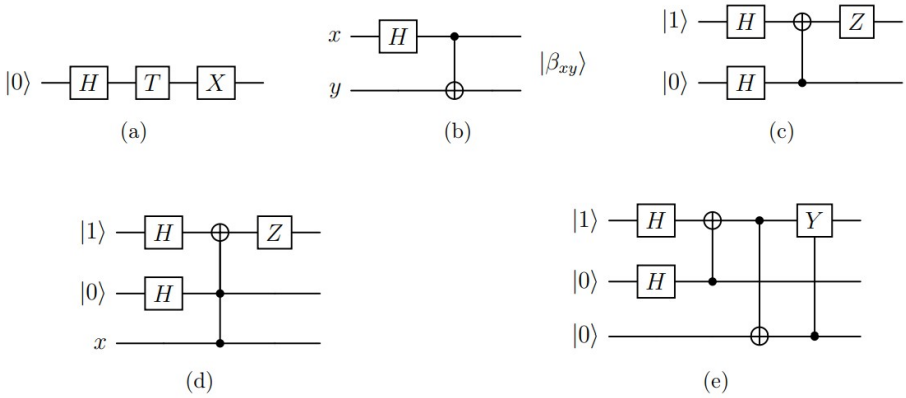
Solution



$$|\psi_1\rangle = |a, a \oplus b\rangle$$
$$|\psi_2\rangle = |a \oplus (a \oplus b), a \oplus b\rangle = |b, a \oplus b\rangle$$
$$|\psi_3\rangle = |b, b \oplus (a \oplus b)\rangle = |b, a\rangle$$

KUL-2023-10.1.2

What are the output states of the following circuits?



Solutions

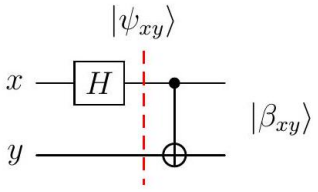
The solutions is generally more easily obtained using the ket representation than the matrix representation (especially for more than 1 qubit). We can then use, for example, that $\hat{H}|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $\hat{H}|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$.

Let's denote the output state as $|\alpha\rangle$.

Solutions to (a)

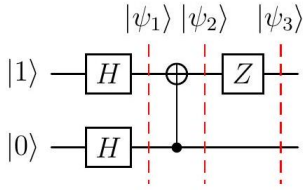
$|\alpha\rangle = \hat{X}\hat{T}\hat{H}|0\rangle = \frac{1}{\sqrt{2}}\left(e^{i\pi/4}|0\rangle + |1\rangle\right)$.

Solutions to (b)



x	y	$\lvert\psi_{xy}\rangle$	$\lvert\beta_{xy}\rangle$
0	0	$\frac{1}{\sqrt{2}}(\lvert00\rangle + \lvert10\rangle)$	$\frac{1}{\sqrt{2}}(\lvert00\rangle + \lvert11\rangle)$
0	1	$\frac{1}{\sqrt{2}}(\lvert01\rangle + \lvert11\rangle)$	$\frac{1}{\sqrt{2}}(\lvert01\rangle + \lvert10\rangle)$
1	0	$\frac{1}{\sqrt{2}}(\lvert00\rangle - \lvert10\rangle)$	$\frac{1}{\sqrt{2}}(\lvert00\rangle - \lvert11\rangle)$
1	1	$\frac{1}{\sqrt{2}}(\lvert01\rangle - \lvert11\rangle)$	$\frac{1}{\sqrt{2}}(\lvert01\rangle - \lvert10\rangle)$

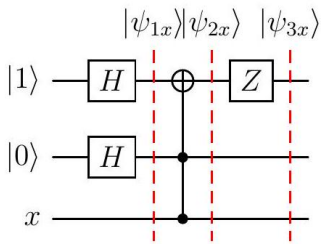
Solutions to (c)



$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) =$$
$$= \frac{1}{2}(|00\rangle + |01\rangle - |10\rangle - |11\rangle)$$
$$|\psi_2\rangle = \frac{1}{2}(|00\rangle + |11\rangle - |10\rangle - |01\rangle)$$
$$|\psi_3\rangle = \frac{1}{2}(|00\rangle + |11\rangle - |10\rangle - |01\rangle)$$

Solutions to (d)

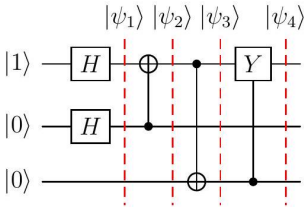
The controlled-NOT with two control qubits (Toffoli gate) applies the NOT if the two control qubits are 1.



$$|\psi_{1x}\rangle = \frac{1}{2}(|00\rangle + |01\rangle - |10\rangle - |11\rangle) \otimes |x\rangle =$$
$$= \frac{1}{2}(|00x\rangle + |01x\rangle - |10x\rangle - |11x\rangle)$$
$$|\psi_{2,x=0}\rangle = \frac{1}{2}(|000\rangle + |010\rangle - |100\rangle - |110\rangle) = |\psi_{1,x=0}\rangle$$
$$|\psi_{2,x=1}\rangle = \frac{1}{2}(|001\rangle + |111\rangle - |101\rangle - |011\rangle)$$
$$|\psi_{3,x=0}\rangle = \frac{1}{2}(|000\rangle + |010\rangle + |100\rangle + |110\rangle)$$
$$|\psi_{3,x=1}\rangle = \frac{1}{2}(|001\rangle - |111\rangle + |101\rangle - |011\rangle)$$

Solutions to (e)

The last gate of the circuit is a controlled- Y gate, i.e. the Y gate is applied only if the control qubit is 1.



$$|\psi_1\rangle = \frac{1}{2}(|000\rangle + |010\rangle - |100\rangle - |110\rangle)$$
$$|\psi_2\rangle = \frac{1}{2}(|000\rangle + |110\rangle - |100\rangle - |010\rangle)$$
$$|\psi_3\rangle = \frac{1}{2}(|000\rangle + |111\rangle - |101\rangle - |010\rangle)$$
$$|\psi_4\rangle = \frac{1}{2}(|000\rangle - i|011\rangle + i|001\rangle - |010\rangle)$$

KUL-2023-10.1.3

Show that if $A^2 = I$ then $\exp(iAx) = \cos(x)I + i\sin(x)A$. Use this result to express the rotation matrix $R_J(\theta) = \exp(-iJ\theta/2)$ with $J = X, Y, Z$ and check that $T = R_z(\pi/4)$ up to a global phase.

Solution

If $A^2 = I$, then we can transform separately contributions from even and odd exponents in the Taylor expansion, since $A^{2n} = I$ and $A^{2n+1} = A$:

$$e^{iAx} = \sum_n \frac{(iAx)^n}{n!} = \sum_n \frac{(ix)^{2n}}{(2n)!} I + \sum_n \frac{(ix)^{2n+1}}{(2n+1)!} A = I \sum_n \frac{(-1)^n (x)^{2n}}{(2n)!} + iA \sum_n \frac{(-1)^n (x)^{2n+1}}{(2n+1)!} = I\cos(x) + iA\sin(x)$$

We can then easily see that $X^2 = I, Y^2 = I$ and $Z^2 = I$, so we have

$$R_z(\theta) = e^{-iZ\theta/2} = \cos\left(\frac{\theta}{2}\right) I - i \sin\left(\frac{\theta}{2}\right) Z = \begin{bmatrix} \cos\left(\frac{\theta}{2}\right) - i\sin\left(\frac{\theta}{2}\right) & 0 \\ 0 & \cos\left(\frac{\theta}{2}\right) + i\sin\left(\frac{\theta}{2}\right) \end{bmatrix} = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}$$

We can then apply a rotation of $\pi/4$ to obtain

$$R_z(\pi/4) = \begin{bmatrix} e^{-i\pi/8} & 0 \\ 0 & e^{i\pi/8} \end{bmatrix} = e^{-i\pi/8} \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix} = e^{-i\pi/8} T$$

KUL-2023-10.2 Quantum Fourier Transform (???)

For a given vector of N complex numbers x_i, the discrete Fourier transform outputs a new vector of N complex numbers $y_k \equiv \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} x_j e^{i2\pi jk/N}$.

The quantum Fourier transform is defined in a similar way. The quantum Fourier transform in an orthonormal basis $|0\rangle, |1\rangle, ..., |N-1\rangle$ is the linear operator such that, for a basis vector,

$$|j\rangle \longrightarrow \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{i2\pi jk/N} |k\rangle$$

and for an arbitrary state, we can write

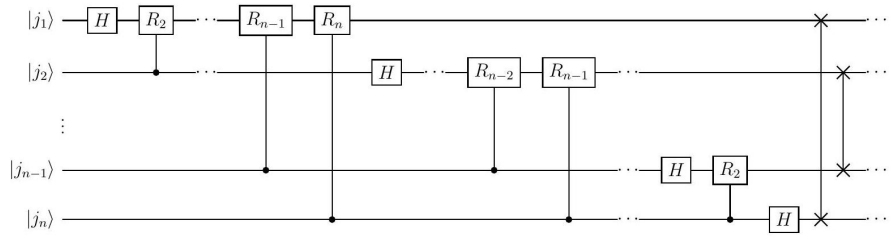
$$\sum_{j=0}^{N-1} x_j|j\rangle \longrightarrow \sum_{k=0}^{N-1} y_k|k\rangle$$

where the y_k are the discrete Fourier transform of the x_j. Moreover, it can be shown to be unitary.

The trick to design a quantum circuit able to perform this unitary transformation is to notice that it can be rewritten using products of states. We consider $N = 2^n$ so that the basis $|0\rangle, |1\rangle, ..., |2^n - 1\rangle$ forms a basis for n qubits. Each state $|j\rangle$ is then represented by $|j_1, ..., j_n\rangle$ where the binary numbers j_k form the representation of the number j in the binary basis, i.e. $j = j_1 2^{n-1} + j_2 2^{n-2} + \cdots + j_{n-1}2^1 + j_n 2^0$. Each state $|j_k\rangle$ is thus the state of a qubit. We also use the notation $0.j_l j_{l+1} ... j_m$ for a binary fraction $j_l 2^{-1} + j_{l+1}2^{-2} + \cdots + j_m 2^{l-m-1}$. It can then be shown that the product representation of the quantum Fourier transform of a basis state is

$$|j_1, ..., j_n\rangle \longrightarrow \frac{\left(|0\rangle + e^{2\pi i 0 \cdot j_n}|1\rangle\right)\left(|0\rangle + e^{2\pi i 0 \cdot j_{n-1} j_n}|1\rangle\right) \cdots \left(|0\rangle + e^{2\pi i 0 . j_1 j_2 \cdots j_n}|1\rangle\right)}{2^{n/2}}$$

From this representation, we can design a quantum circuit that will perform the quantum Fourier transformation:



$$R_k \equiv \begin{bmatrix} 1 & 0 \\ 0 & e^{2\pi i/2^k} \end{bmatrix}$$

We will break it down to check that it indeed does what it is supposed to do.

(a) Check that the Hadamard gate applied on a qubit $|j_k\rangle$ can be written

$$|j_k\rangle \longrightarrow \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i\pi j_k}|1\rangle\right) = \frac{1}{\sqrt{2}}\left(|0\rangle + e^{2\pi i 0 \cdot j_k}|1\rangle\right)$$

(b) Check that the controlled-R_3 gate changes a target qubit $|0\rangle$ into $|0\rangle$ and $|1\rangle$ into $e^{2\pi i 0.00 j_l}|1\rangle$ if the control qubit is $|j_l\rangle$.

(c) What is then the state $|j_k\rangle$ after a Hadamard gate and the controlled- R_2 gate with control qubit $|j_{k+1}\rangle$?

d) Write the state of a qubit $|j_k\rangle$ before the swaps.

As a result, after the swap, we retrieve as output exactly the formula of the quantum Fourier transform, i.e.

$$\frac{\left(|0\rangle + e^{2\pi i 0 \cdot j_n}|1\rangle\right)\left(|0\rangle + e^{2\pi i 0 \cdot j_{n-1} j_n}|1\rangle\right) \cdots \left(|0\rangle + e^{2\pi i 0 . j_1 j_2 \cdots j_n}|1\rangle\right)}{2^{n/2}}$$

Solutions to (a)

We need to check that $\hat{H}|j_k\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i\pi j_k}|1\rangle\right)$. By definition of H, we have

$$\hat{H}|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$
$$\hat{H}|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

In our case, if $j_k = 0$, we get $e^{i\pi j_k} = e^0 = 1$ and get the expected results, and if $j_k = 1$, we have $e^{i\pi j_k} = e^{i\pi} = -1$, and we also get the expected result. In the binary basis and with our notation, we can write j_k as $2 \cdot 0.j_k$ (since $j_k = j_k \cdot 2^0$ and $0.j_k = j_k \cdot 2^{-1}$), so we can indeed write

$$\hat{H}|j_k\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i\pi j_k}|1\rangle\right) = \frac{1}{\sqrt{2}}\left(|0\rangle + e^{2\pi i 0 . j_k}|1\rangle\right)$$

Solutions to (b)

With a controlled- R_3 (CR_3), the target qubit remains unchanged if the control qubit is 0. As a result, writing first the target qubit, then the control qubit, we have $C\hat{R}_3|x,0\rangle = |x,0\rangle$. If the control qubit is 1, then we have

$$C\hat{R}_3|0,1\rangle = |0,1\rangle$$
$$C\hat{R}_3|1,1\rangle = e^{2\pi i/8}|1,1\rangle$$

We must now check that $|0\rangle$ is always transformed into $|0\rangle$, which is straightforward from the relations above, and that $|1\rangle$ is transformed into $e^{2\pi i 0.00 j_l}|1\rangle$. If $j_l = 0$, then we get $|1\rangle \to e^0|1\rangle = |1\rangle$, as expected. If $j_l = 1$, we get

$$|1\rangle \to e^{2\pi i \cdot 0.001}|1\rangle = e^{2\pi i \cdot 2^{-3}}|1\rangle = e^{2\pi i/8}|1\rangle$$

again as expected. We can then notice that for a controlled- R_2 gate, we would get a factor $e^{2\pi i j_l \cdot 2^{-2}} = e^{2\pi i \cdot 0.0 j_l}$, and for a controlled- $R_2 e^{2\pi i j_l \cdot 2^{-n}} = e^{2\pi i \cdot 0.0000 \ldots j_l}$

Solutions to (c)

We consider the state (target qubit, control qubit) $|j_k, j_{k+1}\rangle$. Using 1., the Hadamard gate will transform it into

$$\hat{H}|j_k, j_{k+1}\rangle = \frac{|0, j_{k+1}\rangle + e^{2\pi i 0.j_k}|1, j_{k+1}\rangle}{\sqrt{2}}$$

Then, from 2., we have that $|0\rangle$ will remain unchanged after the CR_2 gate, and $|1\rangle$ will be multiplied by a certain factor. We have

$$\begin{aligned} C\hat{R}_2\left(\left(\hat{H}|j_k\rangle\right)\otimes|j_{k+1}\rangle\right) &= \frac{CR_2|0, j_{k+1}\rangle + e^{2\hat{\pi} i 0.j_k}\hat{}\,|1, j_{k+1}\rangle}{\sqrt{2}} \\ &= \frac{|0, j_{k+1}\rangle + e^{2\pi i 0.j_k} e^{2\pi i 0.0 j_{k+1}}|1, j_{k+1}\rangle}{\sqrt{2}} \\ &= \frac{|0, j_{k+1}\rangle + e^{2\pi i 0.j_k j_{k+1}}|1, j_{k+1}\rangle}{\sqrt{2}} \\ &= \frac{|0\rangle + e^{2\pi i 0.j_k j_{k+1}}|1\rangle}{\sqrt{2}}|j_{k+1}\rangle \end{aligned}$$

since $0.j_k + 0.0j_{k+1} = j_k \cdot 2^{-1} + j_{k+1} \cdot 2^{-2} = 0.j_k j_{k+1}$. Note that the control qubit does not change after the whole process.

Solutions to (d)

According to Fig. 2, a qubit $|j_k\rangle (1 \leq k < n)$ will undergo the transformation H followed by CR_2 (control qubit j_{k+1}), then CR_3 (control qubit j_{k+2}), and so on up to
CR_{n-k+1} (control qubit j_n). Let us consider the full state $|j_1, ..., j_n\rangle$. We thus have that the circuit before the swaps acts on a qubit $|j_k\rangle$ as

$$|j_1, ..., j_{k-1}\rangle \otimes \left(C\hat{R_{n-k+1}} ... C\hat{R}_3 C\hat{R}_2\left(\left(\hat{H}|j_k\rangle\right)\otimes|j_{k+1}, ..., j_n\rangle\right)\right)$$

Let us take it step by step. We already know that $C\hat{R}_2\left(\left(\hat{H}|j_k\rangle\right)\otimes|j_{k+1}\rangle\right) = \frac{|0\rangle + e^{2\pi i 0.j_k j_{k+1}}|1\rangle}{\sqrt{2}}|j_{k+1}\rangle$. With the same reasoning as for 3., we can deduce that

$$C\hat{R}_3 C\hat{R}_2\left(\left(\hat{H}|j_k\rangle\right)\otimes|j_{k+1}, j_{k+2}\rangle\right) = \frac{|0\rangle + e^{2\pi i 0.j_k j_{k+1} j_{k+2}}|1\rangle}{\sqrt{2}}|j_{k+1}, j_{k+2}\rangle$$

Applying again the same reasoning for all the remaining gates, we get

$$C\hat{R_{n-k+1}} ... C\hat{R}_3 C\hat{R}_2\left(\left(\hat{H}|j_k\rangle\right)\otimes|j_{k+1}, ..., j_n\rangle\right) = \frac{|0\rangle + e^{2\pi i 0.j_k j_{k+1} ... j_n}|1\rangle}{\sqrt{2}}|j_{k+1}, ..., j_n\rangle$$

or discarding all the control qubits

$$|j_k\rangle \rightarrow \frac{|0\rangle + e^{2\pi i 0 \cdot j_k j_{k+1} \cdots j_n}|1\rangle}{\sqrt{2}}$$

Note that to get the final output, we perform the above transformation for all k and we get

$$|j_1, ..., j_n\rangle \rightarrow \frac{|0\rangle + e^{2\pi i 0.j_1 j_2 ... j_n}|1\rangle}{\sqrt{2}} \frac{|0\rangle + e^{2\pi i 0.j_2 j_3 ... j_n}|1\rangle}{\sqrt{2}} \cdots \frac{|0\rangle + e^{2\pi i 0.j_n}|1\rangle}{\sqrt{2}}$$

The swap operations in the end will reverse the order to get the Quantum Fourier Transform.

Part VI
Special Topics in a Nutshell

21 Other Theories

21.1 Other details of typical methods

21.1.1 Typical Scattering: Details

1D Scatterings: Features and examples

(допишу скоро!)

Scattering of fast particles in 1D

(тут про то, что если быстрые частицы?)
for now see
https://physicspages.com/pdf/Quantum%20mechanics/Born%20approximation%20in%20one%20dimension.pdf

Типичные модели рассеяния 2D

2D Scatterings: Features and examples

Formulas for 2D scattering

$$\hat{H} = -\frac{\hbar^2}{2\mu}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right) + U(\rho)$$
$$\psi^+_{\mathbf{k}}(\boldsymbol{\rho}) \approx e^{ik\rho\cos\varphi} + \sqrt{i}\frac{f(k,\varphi)}{\sqrt{\rho}}e^{ik\rho}, \quad \rho\to\infty$$

(!!! тут про функцию Грина и функцию Генкеля, ее свойства!!!)

$$H_0^{(1)}(x) \approx -(2i/\pi)\log(2i/\gamma x), \quad |x| \ll 1$$

where $\gamma = e^C$ and C is Euler's constant (see Landau)

Примем, что: (?? это пока не могу вывести, в теории напишу про это)

$$G^{(0,R)}_{E\ 2D}(\mathbf{r},\mathbf{r}') = \frac{m}{\sqrt{2\pi k_E r}}e^{ik_E|\mathbf{r}-\mathbf{r}'|+i\frac{\pi}{4}}$$

$$\begin{aligned}\chi_{\mathbf{k}2D}(\mathbf{r}) &= \int d\mathbf{r}'\frac{d\mathbf{k}'}{(2\pi)^2}G^{(0,R)}_{E\ 2D}(\mathbf{r},\mathbf{r}')\ e^{i\mathbf{k}'\mathbf{r}'}\ \langle\mathbf{k}'|\hat{V}|\mathbf{k}\rangle = \\ &= \frac{m}{\sqrt{2\pi kr}}\int d\mathbf{r}'\delta(\mathbf{r}')e^{ik|\mathbf{r}-\mathbf{r}'|+i\frac{\pi}{4}}e^{i\mathbf{k}'\mathbf{r}'}\tilde{V}_{\mathbf{k}-\mathbf{k}'} = \\ &= \frac{m}{\sqrt{2\pi kr}}e^{ikr+i\frac{\pi}{4}}\tilde{V}_{\mathbf{k}-\mathbf{k}'}\end{aligned}$$

$$f_{2D}(\mathbf{n},\mathbf{n}') = \frac{m}{\sqrt{2\pi k}}\tilde{V}_{\mathbf{k}-\mathbf{k}'}$$

$$d\sigma_{2D} = |f(\mathbf{n}, \mathbf{n}')|^2 d\theta$$

(тут про то, что если медленные частицы?)

(тут про то, что если быстрые частицы?)

$$e^{ik\rho\cos\varphi} = \sum_{m=-\infty}^{\infty} A_m J_{|m|}(k\rho) e^{im\varphi}, \quad \psi^+_{\mathbf{k}} = \sum_{m=-\infty}^{\infty} B_m R_{km}(\rho) e^{im\varphi}$$

$$R_{km2D}(\rho) = \sqrt{\frac{2}{\pi k\rho}} \sin\left(k\rho - \frac{\pi|m|}{2} + \frac{\pi}{4} + \delta_m\right)$$

$$f_{2D}(k,\varphi) = \frac{1}{i\sqrt{2\pi k}} \sum_{m=-\infty}^{\infty} \left(e^{2i\delta_m} - 1\right) e^{im\varphi}$$

$$\sigma_{\text{tot}2D} = \int_0^{2\pi} |f|^2 d\varphi = \frac{4}{k} \sum_{m=-\infty}^{\infty} \sin^2\delta_m$$

$$\operatorname{Im} f(k, \varphi = 0) = \sqrt{\frac{k}{8\pi}}\sigma(E). \qquad \text{opt th 2D}$$

Features of 2d scattering

(emphasis main statements, what works here, what is wrong here)
Особенности 2D случая:

$$\psi_{2D}(\mathbf{r}) = e^{i\mathbf{kr}} + f(\mathbf{n}, \mathbf{n}') e^{\frac{i\pi}{4}} \frac{e^{ikr}}{\sqrt{r}}$$

(??? почему???)

3D Scatterings: Features and examples

Scattering on a 3d hard sphere (elastic bounce back):

$$R_l(r) = A_l \left[\cos\alpha_l j_l(\rho) - \sin\alpha_l n_l(\rho)\right]$$

$$R_l(r) \sim \frac{1}{\rho}\left[\cos\alpha_l \sin\left(\rho - \frac{1}{2}l\pi\right) + \sin\alpha_l \cos\left(\rho - \frac{1}{2}l\pi\right)\right] = \frac{1}{\rho}\sin\left(\rho - \frac{1}{2}l\pi + \alpha_l\right) \equiv$$

$$\equiv \sim \left[(-1)^{l+1}\frac{e^{-i\rho}}{\rho} + e^{2i\delta_l}\frac{e^{i\rho}}{\rho}\right] = \frac{e^{i\delta_l}e^{i\pi l/2}}{\rho}\left[-e^{-i(\rho+\delta_l-\pi l/2)} + e^{i(\rho+\delta_l-\pi l/2)}\right]$$

$$\alpha_l = \delta_l$$

$$R_l(a) = 0 \qquad \Rightarrow \qquad \cos\delta_l j_l(ka) = \sin\delta_l n_l(ka) \qquad \Rightarrow \qquad \tan\delta_l = \frac{j_l(ka)}{n_l(ka)}$$

$$\delta_0 = -ka$$

$$\delta_l^{ka\ll 1} \approx -\frac{(ka)^{2l+1}}{(2l+1)!!(2l-1)!!} \qquad j_l(\rho) \overset{\rho\to 0}{\to} \frac{\rho^l}{(2l+1)!!};$$
$$n_l(\rho) \overset{\rho\to 0}{\to} -(2l-1)!!\rho^{-(l+1)}$$

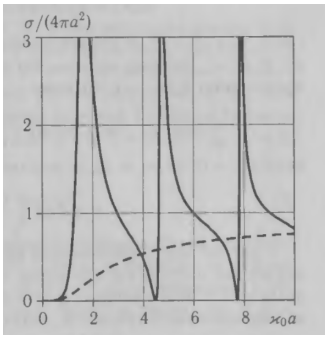
$$\sigma_l^{ka\ll 1} \approx 4\pi a^2\left(1+\mathcal{O}\left((ka)^4\right)\right) \qquad \sigma = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\delta_l$$

This is a factor of 4 bigger than the classical, geometric result.

Scattering on a 3d black sphere (absorption, elastic and inelastic):
(??? what are boundary conditions for this model???)

Эффект Рамзауэра

Медленные частицы рассеиваются на сферически-симметричной прямоугольной потенциальной яме с пиками и нулями в сечении при некоторых соотношениях между глубиной V_0 и радиусом ямы a:



(коротко, почему? см. задачу, это еще продумать нужно)

(строчка про эксп подтверждения)

Поляризуемость связанного состояния диаграммным методом

Пусть заряженная частица находится в мелкой 2D яме в основном состоянии во слабом внешнем поле.

$G = G_0 + G_0 F G_0$,

$$G(\varepsilon, \mathbf{p}, \mathbf{p}') = (2\pi)^2 \frac{\delta^{(2)}(\mathbf{p}-\mathbf{p}')}{\varepsilon - p^2/(2m) + i\delta} + \frac{F(\varepsilon)}{[\varepsilon - p^2/(2m) + i\delta]\,[\varepsilon - p'^2/(2m) + i\delta]}.$$

Положительный знак мнимой части $i\delta$ означает, что состояния непрерывного спектра пусты. При интегрировании по ε эти полюсы надо обходить сверху. Осталось выбрать обход полюса в $F(\varepsilon)$ при $\varepsilon = \varepsilon_0$. Это состояние заполнено, поэтому сдвигаем полюс вверх: $\varepsilon_0 \to \varepsilon_0 + i\delta$. Получаем $F(\varepsilon) = 2\pi\hbar^2/\left(m\ln\left(\varepsilon/\varepsilon_0\right)\right)$, причем обход полюса $\varepsilon = \varepsilon_0$ и точки ветвления $\varepsilon = 0$ такой:

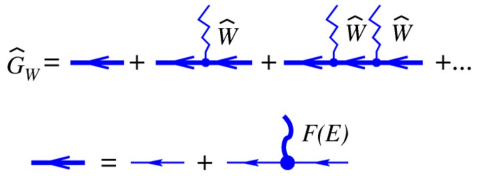
$$\mathcal{P} := e\int \mathbf{r}n(\mathbf{r})d^2r = -ie\int \lim_{t\to-0}\mathbf{r}G(t,\mathbf{r},\mathbf{r})d^2r =$$
$$= e\iint\left(\int \mathbf{r}e^{i(\mathbf{p}_1-\mathbf{p}_2)\mathbf{r}}d^2r\right)\cdot\left(\lim_{t\to-0}\int e^{-i\omega t}G\left(\omega,\mathbf{p}_1,\mathbf{p}_2\right)\frac{d\omega}{2\pi i}\right)\frac{d^2p_1d^2p_2}{(2\pi)^4} =$$
$$= -ie\iint\nabla_1\delta\left(\mathbf{p}_1-\mathbf{p}_2\right)\sum \mathrm{Res}_\omega\, G\left(\omega,\mathbf{p}_1,\mathbf{p}_2\right)\frac{d^2p_1d^2p_2}{(2\pi)^2},$$

(??????????) тут вычеты в полюсах ω функции G в верхней полуплоскости ε, что соответствует заполненным уровням.

$$\mathcal{P} \overset{\text{int b p}}{=} ie\int\left[\nabla_{\mathbf{p}}\sum \mathrm{Res}_\omega\, G\left(\omega,\mathbf{p},\mathbf{p}'\right)\right]\Big|_{\mathbf{p}'=\mathbf{p}}\frac{d^2p}{(2\pi)^2}.$$

Пусть есть поле $W=-eEx$, тогда

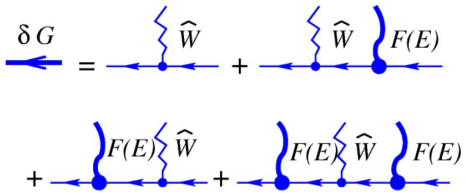
$$\hat{G}_W = \hat{G}+\hat{G}\hat{W}\hat{G}+\hat{G}\hat{W}\hat{W}\hat{G}+\ldots$$



$$W(\mathbf{p}) = -\int eExe^{-i\mathbf{pr}}d^2r = -ie(2\pi)^2E\frac{\partial}{\partial p_x}\delta^{(2)}(\mathbf{p}).$$

Линейный по полю и требуемый для поляризуемости ряд имеет 4 члена:

$$G = G_0+G_0FG_0,$$



1) $G_0WG_0=0$. (нет особенностей над контуром интегрирования по E.)

2) $$\hat{G}_0W\hat{G}_0\hat{F}\hat{G}_0\left(p,p'\right) = \int\frac{-ieE\partial/\partial p_x\delta^{(2)}\left(\mathbf{p}-\mathbf{p}_1\right)}{\left(\varepsilon-p^2/2m+i\delta\right)}\frac{F(\varepsilon)}{\left(\varepsilon-p_1^2/2m+i\delta\right)\left(\varepsilon-p^2/2m+i\delta\right)}d^2\mathbf{p}_1 =$$
$$= \int\delta\left(\mathbf{p}_1-\mathbf{p}\right)\frac{\partial}{\partial p_{1x}}\frac{-ieEF(\varepsilon)}{\left(\varepsilon-p^2/2m+i\delta\right)}\frac{1}{\left(\varepsilon-p_1^2/2m+i\delta\right)\left(\varepsilon-p^2/2m+i\delta\right)}d^2\mathbf{p}_1 =$$
$$= -\frac{ieE}{m}F(\varepsilon)\frac{p_x}{\left(\varepsilon-p^2/2m+i\delta\right)^3\left(\varepsilon-p^2/2m+i\delta\right)}.$$

3) $$\hat{G}_0\hat{F}\hat{G}_0\hat{W}\hat{G}_0\left(\mathbf{p},\mathbf{p}'\right) = \frac{ieEp'_xF(\varepsilon)/m}{\left(\varepsilon-p^2/2m+i\delta\right)\left(\varepsilon-p'^2/2m+i\delta\right)^3}.$$

c.c., $p\leftrightarrow p'$

4) $$\hat{G}_0\hat{F}\hat{G}_0\hat{W}\hat{G}_0\hat{F}\hat{G}_0\left(p,p'\right) =$$
$$= ieEF^2(\varepsilon)\iint\frac{d^2p_1d^2p_2}{(2\pi)^2}G_0(\varepsilon,\mathbf{p})G_0\left(\varepsilon,\mathbf{p}_2\right)G_0\left(\varepsilon,\mathbf{p}_1\right)G_0\left(\varepsilon,\mathbf{p}'\right)\nabla_{1x}\delta\left(\mathbf{p}_2-\mathbf{p}_1\right) =$$
$$= -ieEF^2(\varepsilon)G_0(\varepsilon,p)G_0\left(\varepsilon,\mathbf{p}'\right)\int\frac{d^2p_1}{(2\pi)^2}\frac{p_{1,x}/m}{\left(\varepsilon-p_1^2/2m+i\delta\right)^3} = 0, \quad \text{(odd f)}$$

Итог:

$$\sum_{\omega} \operatorname{Res} G(\omega, \mathbf{p}, \mathbf{p}') = \operatorname{Res}_{\varepsilon_0} F(\varepsilon) \frac{ie}{m} E \left[p'_x G_0(\varepsilon_0, \mathbf{p}) G_0^3(\varepsilon_0, \mathbf{p}') - p_x G_0^3(\varepsilon_0, \mathbf{p}) G_0(\varepsilon_0, \mathbf{p}') \right]$$

$$\mathcal{P}_x = -2 \frac{e^2}{m^2} E \int \frac{p_x^2}{\left(\varepsilon_0 - p^2/2m + i\delta\right)^5} \operatorname{Res}_{\varepsilon_0} F(\varepsilon) \frac{d^2p}{(2\pi)^2}.$$

Итак, поляризуемость:

$$\chi_{\alpha\beta} = \frac{2e^2}{m^2} \int \frac{p_\alpha p_\beta (2m)^5}{\left(p^2 + \varkappa^2\right)^5} \operatorname{Res}_{\varepsilon_0} F(\varepsilon) \frac{d^2p}{(2\pi)^2}, \qquad \varkappa^2 := 2m\,|\varepsilon_0|$$

$$\varepsilon = \varepsilon_0 + z \qquad F(\varepsilon) = \frac{2\pi}{m \ln(1 + z/\varepsilon_0)} \approx \frac{2\pi\varepsilon_0}{mz}, \quad \Rightarrow \quad \operatorname{Res} = \frac{2\pi\varepsilon_0}{m}.$$

$$\chi_{\alpha\beta} = e^2 m^2 \varepsilon_0 \int_0^{+\infty} \frac{2^6 \pi \delta_{\alpha\beta}}{\left(p^2 + \varkappa^2\right)^5} \frac{p^3 dp}{2\pi} = \delta_{\alpha\beta} \frac{16 e^2 m^2 \varepsilon_0}{(2m\varepsilon_0)^3} \int_0^{+\infty} \frac{x dx}{(x+1)^5} = \frac{e^2 \delta_{\alpha\beta}}{6 m \varepsilon_0^2} \cdot \hbar^2.$$

General features of scattering formalisms

Properties of scattering amplitudes

$$f(\mathbf{k}, \mathbf{k}_0) - f^*(\mathbf{k}_0, \mathbf{k}) = \frac{ik}{2\pi} \int f(\mathbf{k}', \mathbf{k}_0) f^*(\mathbf{k}', \mathbf{k}) \, d\Omega' \tag{XIII.26}$$

(For $\mathbf{k} = \mathbf{k}_0$, the optical theorem is reproduced.)

$$f(E, 0) = f^B(0) + \sum_n \frac{d_n}{E - E_n} + \frac{1}{\pi} \int_0^{\infty} \frac{\operatorname{Im} f(E', 0)}{E' - E} dE' \tag{XIII.27}$$

The energy has the following singular points: branch points $E = 0$ and $E = \infty$ and poles E_n on real half-axis $E < 0$, which coincide with the positions of discrete levels.

Here, $f^B(0)$ is the amplitude of the first Born approximation; see Eq. (XIII.6). The summation is performed over all the discrete states in the potential (each of which corresponds to a pole in the scattering amplitude); d_n is the residue at the pole corresponding to E_n, and is given by

$$d_n = -(-1)^{l_n} (2l_n + 1) \frac{\hbar^2 A_n^2}{2m} \tag{XIII.28}$$

where A_n is a normalization coefficient for the large-distance asymptote of the radial wave-function corresponding to a bound state with the angular momentum l_n; that is, $rR_n \approx A_n \exp\{-\kappa_n r\}$ (compare to Eq. (XI.5)).

Extra properties of S-matrix

$$\begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix} = \begin{pmatrix} I_R \\ I_L \end{pmatrix} + S \begin{pmatrix} O_R \\ O_L \end{pmatrix}, \quad S = \begin{pmatrix} t & r \\ r' & t' \end{pmatrix}$$

(????? I don't get the idea of parity basis and all things here by Tong)

For a general parity-symmetric potential $V(x) = V(-x)$. we switch to a parity basis,

$$I_+(x) = e^{-ik|x|}, \quad I_-(x) = \text{sign}(x)e^{-ik|x|}, \quad O_+(x) = e^{ik|x|}, \quad O_-(x) = -\,\text{sign}(x)e^{ik|x|}$$

$$\begin{pmatrix} I_+ \\ I_- \end{pmatrix} = M\begin{pmatrix} I_R \\ I_L \end{pmatrix}, \quad \begin{pmatrix} O_+ \\ O_- \end{pmatrix} = M\begin{pmatrix} O_R \\ O_L \end{pmatrix}, \quad M = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

$$S^P = MSM^{-1}.$$

- For a parity-symmetric potential, $r = r'$ because $\psi_R(x) = \psi_L(-x)$. Then S^P simplifies to

$$S^P = \begin{pmatrix} S_{++} & \\ & S_{--} \end{pmatrix}, \quad S_{++} = t + r, \quad S_{--} = t - r$$

The off-diagonal elements are zero because parity is conserved. - Combining our identities shows that $S_{++}$and $S_{--}$are phases,

$$S_{++} = e^{2i\delta_+(k)}, \quad S_{--} = e^{2i\delta_-(k)}$$

This is analogous to how we distilled three-dimensional central force scattering into a set of phases in the partial wave decomposition. - The S-matrix can also detect bound states. Since the algebra used to derive $r(k)$ and $t(k)$ never assumed that k was real, the same expressions hold for general complex k. Consider a pure imaginary wavenumber $k = i\lambda$ with even parity,

$$\lim_{|x|\to\infty} \psi_+(x) = I_+(x) + S_{++}O_+(x), \quad I_+(x) = e^{\lambda|x|}, \quad O_+(x) = e^{-\lambda|x|}$$

It looks like there can't be a bound state solution here, since the I_+component diverges at infinity. The trick is to rewrite this as

$$\lim_{|x|\to\infty} \psi_+(x) = S_{++}^{-1}I_+(x) + O_+(x)$$

which gives a valid bound state as long as $S_{++}^{-1} = 0$, which corresponds to a pole in S_{++}. That is, we can identify bound states from poles in S-matrix elements! (The same reasoning works in the original left/right basis, though there are more terms.)

$$S_{++}(k) = -e^{-ika}\frac{q\tan(qa/2) - ik}{q\tan(qa/2) + ik}$$

which shows that bound states of even parity occur when $\lambda = q\tan(qa/2)$, a familiar result. We can recover the bound state energy from $E = -\hbar^2\lambda^2/2m$.

Типичные модели рассеяния в приложениях

Рассеяние Мотта

Рассеяние Мотта - рассеяние, обусловленное взаимодействием спина заряженной частицы с её орбитальным моментом, возникающим при движении в электрическом поле рассеивающего центра. Характерной особенностью рассеяния Мотта является его асимметрия относительно плоскости, содержащей спин и импульс электрона. Такая асимметрия используется для измерения поляризации электронов.

Дифференциальное сечение упругого рассеяния частицы со спином 1/2 и зарядом e на неподвижном кулоновском центре (атомном ядре) с зарядом Ze выражается:

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{Mott}} = 4\left(Ze^2\right)^2\frac{E^2}{(qc)^4}\left(1 - \beta^2\sin^2\frac{\theta}{2}\right) \qquad \text{(ф Мотта)}$$

где σ - сечение рассеяния, Ω - телесный угол, Z - зарядовое число атомного ядра, e - элементарный электрический заряд, $E = \gamma c^2$ - энергия частицы, $q = 2\gamma v \sin(\theta/2)$ - переданный импульс (тут $\gamma = 1/\sqrt{1-\beta^2}$ - лоренц-фактор частицы, m - масса частицы, v - скорость частицы, c - скорость света), $\beta = v/c, \theta$ - угол рассеяния. Для нерелятивистских частиц $v \ll c$ и формула Мотта переходит в формулу Резерфорда:

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{Rutherford}} = \left(\frac{Ze^2}{2mv^2}\right)^2 \frac{1}{\sin^4(\theta/2)}$$

(допишу что-то)

Резонанс на квазидискретном уровне

(порешаю по МК, впишу на 1/4 страницы суть)

Об эффекте Мессбауэра

(1 страница максимум, что это, и в чем польза?)
Ответ - что фактор Дебая-Уоллера (??)

Об оценках в задачах рассеяния (!?!??)

(тут мб крутые могут быть методы)

О рассеянии заряженных частиц на ядрах по Мигдалу Крайнову

О рассеянии заряженных частиц на атомном ядре по Мигдалу Крайнову

Features of different scatterings

Особенности рассеяния при больших энергиях

(порешаю по МК, впишу на 1/4 страницы суть)

Особенности рассеяния медленных частиц

(см. Ландау 3, там очень мутные методы с делением коэффициентов, раз подумал, не хватило одного раза, пока не могу сказать, какие особенности)
(порешаю по МК, впишу на 1/4 страницы суть)

21.1.2 Special Scatterings

Spin-dependent scattering

(see Galitski!)
The operator describing interaction of a spin-1/2 particle with an external field has the form:

$$\hat{U} = U_0(r) + U_1(r)\hat{\sigma} \cdot \hat{\mathbf{l}}$$

In case of a spin-dependent interaction, the scattering amplitude becomes a matrix, $\hat{f}$, in the spin-basis, whose elements $\chi_f^* \hat{f} \chi_i$ describe the scattering from an initial spin state χ_i into

a final state χ_f. For the scattering of spin- 1/2 particles off of spinless ones and in the case of a parity-conserving interaction,

$$\hat{f} = A(k,\theta) + iB(k,\theta)\boldsymbol{\nu}\cdot\hat{\boldsymbol{\sigma}}, \quad \boldsymbol{\nu} = \frac{[\mathbf{k}_0\times\mathbf{k}]}{|[\mathbf{k}_0\times\mathbf{k}]|} \tag{XIII.22}$$

The factorization of i - convention, it can be different in other conventions.

The differential scattering cross-section summed over the spin states of the scattered particles is given by

$$\frac{d\sigma}{d\Omega} = |A|^2 + |B|^2 + 2\,\mathrm{Im}\,(AB^*)\,\boldsymbol{\nu}\cdot\mathbf{P}_0 \tag{XIII.23}$$

where $\mathbf{P}_0 = 2\chi_i^*\hat{\boldsymbol{\sigma}}\chi_i$ is the polarization vector of the particles before collision. The polarization state of the scattered particles depends on both the interaction and the initial polarization, $\mathbf{P}_0$. If the particles were not polarized before collision, $\mathbf{P}_0 = \mathbf{0}$, then the polarization vector after scattering is

$$\mathbf{P} = \frac{2\,\mathrm{Im}\,(AB^*)}{|A|^2+|B|^2}\boldsymbol{\nu} \tag{XIII.24}$$

As before, Eq. (XIII.22) for the amplitude can be expanded in terms of the partial waves:

$$\begin{aligned} A &= \frac{1}{2ik}\sum_{l=0}^{\infty}\left[(l+1)\left(\exp\left\{2i\delta_l^+\right\}-1\right)+l\left(\exp\left\{2i\delta_l^-\right\}-1\right)\right]P_l(\cos\theta)\\ B &= \frac{1}{2ik}\sum_{l=1}^{\infty}\left(\exp\left\{2i\delta_l^+\right\}-\exp\left\{2i\delta_l^-\right\}\right)\sin\theta P_l'(\cos\theta), \end{aligned} \tag{XIII.25}$$

$\delta_l^{\pm}$ are the phase shifts for states with the orbital angular momentum l and the total angular momentum $j = l \pm 1/2$.

Scattering Off a Lattice

(это же в конд среды добавлю)

Typical formalism

$$\psi(\mathbf{r}) \sim e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R})} + f\left(\mathbf{k},\mathbf{k}'\right)\frac{e^{ik|\mathbf{r}-\mathbf{R}|}}{|\mathbf{r}-\mathbf{R}|}$$

$$|\mathbf{r}-\mathbf{R}| = \sqrt{r^2+R^2-2\mathbf{r}\cdot\mathbf{R}} \approx r\sqrt{1-2\mathbf{r}\cdot\mathbf{R}/r^2} \approx r - \hat{\mathbf{r}}\cdot\mathbf{R}$$

$$\psi(\mathbf{r}) \sim e^{-i\mathbf{k}\cdot\mathbf{R}}\left[e^{i\mathbf{k}\cdot\mathbf{r}} + f\left(\mathbf{k},\mathbf{k}'\right)e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}}\frac{e^{ikr}}{r}\right]$$

$$f_{\mathbf{R}}(\mathbf{k};\hat{\mathbf{r}}) = f\left(\mathbf{k},\mathbf{k}'\right)e^{i\mathbf{q}\cdot\mathbf{R}}$$

$$\mathrm{q} = \mathrm{k} - \mathrm{k}'$$

$$f_{\Lambda}\left(\mathbf{k},\mathbf{k}'\right) = f\left(\mathbf{k},\mathbf{k}'\right)\sum_{\mathbf{R}\in\Lambda}e^{i\mathbf{q}\cdot\mathbf{R}}$$

$$\Delta(\mathbf{q}) \equiv \sum_{\mathbf{R}\in\Lambda} e^{i\mathbf{q}\cdot\mathbf{R}} = \sum_{\mathbf{R}\in\Lambda} e^{i\mathbf{q}\cdot(\mathbf{R}-\mathbf{R}_0)} = e^{-i\mathbf{q}\cdot\mathbf{R}_0}\Delta(\mathbf{q})$$

either $e^{-i\mathbf{q}\cdot\mathbf{R}_0} = 1$ or $\Delta(\mathbf{q}) = 0$.
$\mathrm{q} \in \Lambda^\star$.

$$\sum_{\mathbf{R}\in\Lambda} e^{i\mathbf{q}\cdot\mathbf{R}} \equiv \Delta(\mathbf{q}) = V^\star \sum_{\mathbf{Q}\in\Lambda^*} \delta(\mathbf{q}-\mathbf{Q})$$

$\mathbf{k}-\mathbf{k}' \in \Lambda^\star$ laue condition

(добавлю картинки и пояснения)

The Bragg Condition

$$d = \frac{2\pi}{Q}$$

$$\lambda = 2d\sin(\theta/2)$$

$$n\lambda = 2d\sin(\theta/2)$$

(добавлю картинки и пояснения)

The Structure Factor

$$f_{\text{lattice}}\ (\mathbf{k},\mathbf{k}') = \Delta(\mathbf{q})S(\mathbf{q})$$
$$S(\mathbf{q}) = \sum_i f_i\,(\mathbf{k},\mathbf{k}')\,e^{i\mathbf{q}\cdot\mathbf{d}_i} \quad \text{structure factor.}$$

An Example: BCC Lattice
(??)

Another Example: Diamond
(???)

The Debye-Waller Factor

(абзац с сутью и постановкой задачи!)

$$f_\Lambda\,(\mathbf{k},\mathbf{k}') = f\,(\mathbf{k},\mathbf{k}')\sum_n e^{i\mathbf{q}\cdot\mathbf{R}_n}$$

$$R_n \to R_n + \mathbf{u}_n(t)$$

$$\tilde{\Delta}(\mathbf{q}) = \sum_n e^{i\mathbf{q}\cdot\mathbf{R}_n} e^{i\mathbf{q}\cdot\mathbf{u}_n}$$

$$\tilde{\Delta}(\mathbf{q}) = \sum_n e^{i\mathbf{q}\cdot\mathbf{R}_n}\langle 0|e^{i\mathbf{q}\cdot\mathbf{u}_n(t)}|0\rangle$$

$$u_n(t) = X_0(t) + \sqrt{\frac{\hbar}{2m\omega_l N}} \sum_{l\neq 0} \left[a_l e^{-i(\omega_l t - k_l na)} + a_l^\dagger e^{i(\omega_l t - k_l na)} \right]$$

$$u_0 = \sum_{k\neq 0} \sqrt{\frac{\hbar}{2mN\omega(k)}} \left(a(k) + a^\dagger(k) \right) \equiv A + A^\dagger$$

$$\left[A, A^\dagger \right] = \sum_{k\neq 0} \frac{\hbar}{2mN\omega(k)}$$

$\langle 0 | e^{iq\left(A+A^\dagger\right)} | 0 \rangle$=?

$$e^{iq\left(A+A^\dagger\right)} = e^{iqA^\dagger} e^{iqA} e^{\frac{1}{2}q^2\left[A^\dagger, A\right]}$$

$\langle 0 | e^{i\mathbf{q}\cdot\mathbf{u}_0} | 0 \rangle = e^{-W(\mathbf{q})}$ where $W(\mathbf{q}) = \sum_{\mathbf{k}} \frac{\hbar \mathbf{q}^2}{4mN\omega(\mathbf{k})}$ Debye-Waller factor

$$f_\Lambda\left(\mathbf{k}, \mathbf{k}'\right) = e^{-W(\mathbf{q})} f\left(\mathbf{k}, \mathbf{k}'\right) \Delta(\mathbf{q})$$

21.1.3 Details of typical adiabatics

Адиабатические возмущения по Мигдалу Крайнову

Захват электрона протоном (перезарядка) (89).

О быстрой и медленной подсистемах по Мигдалу Крайнову и приближении Борна-Опенгеймера

(лучше только у МК спишу сперва, по идее у ПТФ это же, потом уже у них буду выписывать это все)

Формализм деления на быстрые и медленные переменные (!!!)

(!! впишу очень скоро!!!)

адиабатический квантовый транспорт

Оценки в адиабатике по МК

Колебательные уровни молекулы

Возбуждение ядерных дипольных уровней быстрой частицей (98).

Рассеяние протона на атоме водорода (перезарядка) (101).

Рождение мягких квантов при рассеянии («инфракрасная катастрофа») (103).

21.1.4 Scattering: Other Details of Basic Methods

Scattering as a time-dependent perturbation by Sakurai

$$U_I(t,t_0) = 1 - \frac{i}{\hbar}\int\limits_{t_0}^{t} V_I(t')\,U_I(t',t_0)\,dt'.$$

$$\langle n\,|U_I(t,t_0)|\,i\rangle = \delta_{ni} - \frac{i}{\hbar}\sum_m \langle n|V|m\rangle \int\limits_{t_0}^{t} e^{i\omega_{nm}t'}\,\langle m\,|U_I(t',t_0)|\,i\rangle\,dt',$$

$\langle n|i\rangle = \delta_{ni}, \quad \hbar\omega_{nm} = E_n - E_m.$

$$\begin{aligned}\langle n\,|U_I(t,t_0)|\,i\rangle &= \delta_{ni} - \frac{i}{\hbar}\langle n|V|i\rangle \int\limits_{t_0}^{t} e^{i\omega_{ni}t'}dt' \\ &= \delta_{ni} - \frac{i}{\hbar}T_{ni}\int\limits_{t_0}^{t} e^{i\omega_{ni}t'+\varepsilon t'}dt'\end{aligned}$$

$$\begin{aligned}S_{ni} := \lim_{t\to\infty}\left[\lim_{\varepsilon\to 0}\langle n\,|U_I(t,-\infty)|\,i\rangle\right] &= \delta_{ni} - \frac{i}{\hbar}T_{ni}\int\limits_{-\infty}^{\infty} e^{i\omega_{nit}t'}dt' \\ &= \delta_{ni} - 2\pi i\delta(E_n - E_i)\,T_{ni}.\end{aligned}$$

$$w(i\to n) = \frac{d}{dt}\left|\langle n\,|U_I(t,-\infty)|\,i\rangle\right|^2,$$

$$\langle n\,|U_I(t,-\infty)|\,i\neq n\rangle = -\frac{i}{\hbar}T_{ni}\int\limits_{-\infty}^{t} e^{i\omega_{ni}t'+\varepsilon t'}dt' = -\frac{i}{\hbar}T_{ni}\frac{e^{i\omega_{ni}t+\varepsilon t}}{i\omega_{ni}+\varepsilon}$$

$$w(i\to n) = \frac{d}{dt}\left[\frac{1}{\hbar^2}|T_{ni}|^2\frac{e^{2\varepsilon t}}{\omega_{ni}^2+\varepsilon^2}\right] = \frac{1}{\hbar^2}|T_{ni}|^2\frac{2\varepsilon e^{2\varepsilon t}}{\omega_{ni}^2+\varepsilon^2}.$$

We need to take $\varepsilon\to 0$ for finite values of t, and then $t\to\infty$. Clearly this will send $w\to 0$ if $\omega_{ni}\neq 0$, so we see something like $\delta(\omega_{ni})$ emerging, which is not unexpected given (6.1.11). In fact, because

$$\int\limits_{-\infty}^{\infty}\frac{1}{\omega^2+\varepsilon^2}d\omega = \frac{\pi}{\varepsilon}$$

$$\lim_{\varepsilon\to 0}\frac{\varepsilon e^{2\varepsilon t}}{\omega_{ni}^2+\varepsilon^2}=\pi\delta\left(\omega_{ni}\right)=\pi\hbar\delta\left(E_n-E_i\right).$$

$$w(i\to n)=\frac{2\pi}{\hbar}\left|T_{ni}\right|^2\delta\left(E_n-E_i\right)$$

$$\Delta n=4\pi|\mathbf{n}|^2\Delta|\mathbf{n}|\times\frac{d\Omega}{4\pi},$$

$$\rho\left(E_n\right)=\frac{\Delta n}{\Delta E_n}=\frac{m}{\hbar^2}\left(\frac{L}{2\pi}\right)^2|\mathbf{n}|d\Omega=\frac{mk}{\hbar^2}\left(\frac{L}{2\pi}\right)^3 d\Omega,$$

$$w(i\to n)=\frac{mkL^3}{(2\pi)^2\hbar^3}\left|T_{ni}\right|^2 d\Omega.$$

$$\mathbf{j}(\mathbf{x},t)=\left(\frac{\hbar}{m}\right)\frac{\mathbf{k}}{L^3}=\frac{v}{L^3}$$

Solving for the T Matrix:

$$\left\langle n\left|U_I(t,-\infty)\right|i\right\rangle=\delta_{ni}+\frac{1}{\hbar}T_{ni}\frac{e^{i\omega_{ni}t+\varepsilon t}}{-\omega_{ni}+i\varepsilon}.$$

$V_{nm}=\langle n|V|m\rangle$,

$$\left\langle n\left|U_I(t,-\infty)\right|i\right\rangle=\delta_{ni}-\frac{i}{\hbar}\sum_m V_{nm}\int_{-\infty}^{t}e^{i\omega_{nm}t'}\left\langle m\left|U_I\left(t',-\infty\right)\right|i\right\rangle dt'.$$

$$-\frac{i}{\hbar}\frac{1}{\hbar}\sum_m V_{nm}\frac{T_{mi}}{-\omega_{mi}+i\varepsilon}\int_{-\infty}^{t}e^{i\omega_{nm}t'+i\omega_{mi}t'+\varepsilon t'}dt'.$$

$$T_{ni}=V_{ni}+\frac{1}{\hbar}\sum_m V_{nm}\frac{T_{mi}}{-\omega_{mi}+i\varepsilon}=V_{ni}+\sum_m V_{nm}\frac{T_{mi}}{E_i-E_m+i\hbar\varepsilon}.$$

$$T_{ni}=\sum_j\langle n|V|j\rangle\left\langle j|\psi^{(+)}\right\rangle=\left\langle n|V|\psi^{(+)}\right\rangle.$$

$$\left\langle n|V|\psi^{(+)}\right\rangle=\langle n|V|i\rangle+\sum_m\langle n|V|m\rangle\frac{\left\langle m|V|\psi^{(+)}\right\rangle}{E_i-E_m+i\hbar\varepsilon}.$$

$$\left|\psi^{(+)}\right\rangle=|i\rangle+\frac{1}{E_i-H_0+i\hbar\varepsilon}V\left|\psi^{(+)}\right\rangle.\qquad\text{Lippmann-Schwinger eq}$$

$$T=V+V\frac{1}{E_i-H_0+i\hbar\varepsilon}T$$

$$T=V+V\frac{1}{E_i-H_0+i\hbar\varepsilon}V+V\frac{1}{E_i-H_0+i\hbar\varepsilon}V\frac{1}{E_i-H_0+i\hbar\varepsilon}V+\cdots.$$

$$G_\pm\left(\mathbf{x},\mathbf{x}'\right)\equiv\frac{\hbar^2}{2m}\left\langle\mathbf{x}\left|\frac{1}{E-H_0\pm i\varepsilon}\right|\mathbf{x}'\right\rangle$$

$$G_\pm\left(\mathbf{x},\mathbf{x}'\right)=\frac{\hbar^2}{2m}\sum_{\mathbf{k}'}\sum_{\mathbf{k}''}\langle\mathbf{x}|\mathbf{k}'\rangle\left\langle\mathbf{k}'\left|\frac{1}{E-H_0\pm i\varepsilon}\right|\mathbf{k}''\right\rangle\langle\mathbf{k}''|\mathbf{x}'\rangle.$$

$$\left\langle \mathbf{k}' \left| \frac{1}{E-(\hbar^2\mathbf{k}'^2/2m)\pm i\varepsilon} \right| \mathbf{k}'' \right\rangle = \frac{\delta_{\mathbf{k}'\mathbf{k}''}}{E-(\hbar^2\mathbf{k}'^2/2m)\pm i\varepsilon}$$

$$\langle \mathbf{x}|\mathbf{k}'\rangle = \frac{e^{i\mathbf{k}'\cdot\mathbf{x}}}{L^{3/2}}$$

$$\text{and} \qquad \langle \mathbf{k}''|\mathbf{x}'\rangle = \frac{e^{-i\mathbf{k}''\cdot\mathbf{x}'}}{L^{3/2}},$$

$E=\hbar^2k^2/2m$.

$$G_\pm(\mathbf{x},\mathbf{x}') = \frac{1}{L^3}\sum_{\mathbf{k}'} \frac{e^{i\mathbf{k}'\cdot(\mathbf{x}-\mathbf{x}')}}{k^2-k'^2\pm i\varepsilon}$$

$$\begin{aligned} G_\pm(\mathbf{x},\mathbf{x}') &= \frac{1}{(2\pi)^3}\int d^3k' \frac{e^{i\mathbf{k}'\cdot(\mathbf{x}-\mathbf{x}')}}{k^2-k^2\pm i\varepsilon} \\ &= \frac{1}{(2\pi)^2}\int\limits_0^\infty k'^2dk' \int\limits_{+1}^{-1} d\mu \frac{e^{ik'|\mathbf{x}-\mathbf{x}'|\mu}}{k^2-k^2\pm i\varepsilon} \\ &= \frac{1}{8\pi^2}\frac{1}{i\,|\mathbf{x}-\mathbf{x}'|}\int\limits_{-\infty}^{\infty} k'dk' \left[\frac{e^{-ik'|\mathbf{x}-\mathbf{x}'|}-e^{ik'|\mathbf{x}-\mathbf{x}'|}}{k^2-k'^2\pm i\varepsilon}\right] \end{aligned}$$

(??? is the formula below useful?)

$$c_n^{(2)} = \frac{i}{\hbar}\sum_m \frac{V_{nm}V_{mi}}{E_m-E_i}\int\limits_0^t dt' \left(e^{i\omega_{nit}t'} - e^{i\omega_{nm}t'}\right)$$

Амплитуда рассеяния в энергетической нормировке и диаграммный ряд для нее

$$\hat{G}^{-1}\psi_{\mathbf{k}}(\mathbf{r}) = 0 \quad \Leftrightarrow \quad \left(\hat{G}_0^{-1}-\hat{V}\right)\psi_{\mathbf{k}}(\mathbf{r}) = 0.$$

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} + \chi_{\mathbf{k}}(\mathbf{r})$$

$$\varepsilon = k^2/2m \qquad \Rightarrow \qquad \left(\hat{G}_0^{-1}-\hat{V}\right)\chi_{\mathbf{k}}(\mathbf{r}) = V|\mathbf{k}\rangle$$

$$\chi_{\mathbf{k}}(\mathbf{r}) = \langle \mathbf{r}|\hat{G}\hat{V}|\mathbf{k}\rangle = \left\langle \mathbf{r}\left|\hat{G}_0\hat{V}+\hat{G}_0\hat{V}\hat{G}_0\hat{V}+...\right|\mathbf{k}\right\rangle.$$

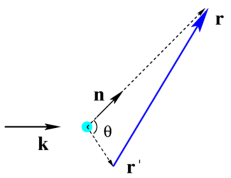
$$\hat{F} := \hat{V}+\hat{V}\hat{G}_0\hat{V}+\hat{V}\hat{G}_0\hat{V}\hat{G}_0\hat{V}+...$$

$\hat{F}$ - т.н. амплитуда рассеяния в энергетической нормировке.

$$\chi_{\mathbf{k}}(\mathbf{r}) = \left\langle \mathbf{r}\left|\hat{G}_0\hat{F}\right|\mathbf{k}\right\rangle.$$

$\hat{F}$ описывает многократное рассеяние падающей волны на потенциале $V(\mathbf{r})$, а $\hat{G}_0$ - свободное движение после последнего рассеяния.

$$G_0(\varepsilon,\mathbf{r},\mathbf{r}') = \int \frac{e^{i\mathbf{p}(\mathbf{r}-\mathbf{r}')}}{\varepsilon-\mathbf{p}^2/2m+i\delta}\frac{d^3p}{(2\pi)^3} = -\frac{m}{2\pi\hbar^2}\frac{e^{i\varkappa|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}, \qquad \hbar\varkappa = \sqrt{2m\varepsilon}$$

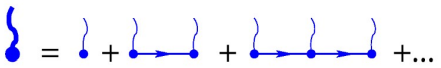


$\mathbf{r} \equiv R\mathbf{n}$, $|\mathbf{r}-\mathbf{r}'| = R - |\mathbf{r}'|\cos\theta + O(1/R)$,

$$\chi_{\mathbf{k}}(\mathbf{r}) = \left\langle \mathbf{r}\left|\hat{G}_0\hat{F}\right|\mathbf{k}\right\rangle = -\frac{m}{2\pi\hbar^2}\frac{e^{i\varkappa R}}{R}\int e^{-i\varkappa|\mathbf{r}'|\cos\theta}\,\langle\mathbf{r}'|F|\mathbf{k}\rangle\,d^3r'$$

$$f(\mathbf{k}_1,\mathbf{k}_2) := -\frac{m}{2\pi\hbar^2}\left\langle \mathbf{k}_2|\hat{F}|\mathbf{k}_1\right\rangle \qquad \text{def}, \quad \mathbf{k}_2 := |k_1|\,\mathbf{n}$$

Рассеяние частицы в статическом $V(\mathbf{r})$ описывается так:



$$\widehat{F} = \widehat{V} + \widehat{V}\widehat{G}_0\widehat{V} + \widehat{V}\widehat{G}_0\widehat{V}\widehat{G}_0\widehat{V} + \ldots = \widehat{V} + \widehat{V}\widehat{G}_0\left(\widehat{V} + \widehat{V}\widehat{G}_0\widehat{V} + \ldots\right) = \widehat{V} + \widehat{V}\widehat{G}_0\widehat{F}$$

$$F(\mathbf{k}_1,\mathbf{k}_2) = F^{(1)}(\mathbf{k}_1,\mathbf{k}_2) + F^{(2)}(\mathbf{k}_1,\mathbf{k}_2) + \ldots,$$

$F^{(1)}(\mathbf{k}_1,\mathbf{k}_2) = V(\mathbf{k}_2-\mathbf{k}_1)$,

$F^{(2)}(\mathbf{k}_1,\mathbf{k}_2) = \int \dfrac{V(\mathbf{k}_2-\mathbf{q})\,V(\mathbf{q}-\mathbf{k}_1)\,(d^3q)}{\varepsilon - \mathbf{q}^2/(2m) + i\delta}$,

$F^{(n)}(\mathbf{k}_1,\mathbf{k}_2) = \int\ldots\int \dfrac{V(\mathbf{k}_2-\mathbf{q}_{n-1})\ldots V(\mathbf{q}_1-\mathbf{k}_1)\,(d^3q_{n-1})\ldots(d^3q_1)}{\left(\varepsilon-\mathbf{q}_{n-1}^2/(2m)+i\delta\right)\ldots\left(\varepsilon-\mathbf{q}_1^2/(2m)+i\delta\right)} \qquad (d^3q_i) := d^3q_i/(2\pi)^3,\ \varepsilon := \hbar^2\mathbf{k}_1^2/(2m)$

$$F(\mathbf{k}_1,\mathbf{k}_2) = V(\mathbf{k}_2-\mathbf{k}_1) + \frac{2m}{\hbar^2}\int \frac{V(\mathbf{k}_2-\mathbf{q})\,F(\mathbf{k}_1,\mathbf{q})}{k_1^2-q^2+i\delta}\frac{d^3q}{(2\pi)^3}.$$

Полюсы $G(\varepsilon)$ дают спектр системы, и так как $\widehat{G} = \widehat{G}_0 + \widehat{G}_0\widehat{F}\widehat{G}_0$, каждому связанному состоянию отвечает полюс $\widehat{F}(\varepsilon)$.

Coulomb scattering

Main formulas for Coulomb scattering

(берем просто предел для Юкавы и всё)
(из ЛЛ3 самые важные выпишу!)

Coulomb scattering by Tong

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{A}{r}\right)\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

$$\left(\nabla^2 + k^2 - \frac{2\gamma k}{r}\right)\psi(\mathbf{r}) = 0$$

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}+k^2-\frac{l(l+1)}{r^2}-\frac{2\gamma k}{r}\right)R_l(r)=0$$

$$R_l(r)\sim\frac{e^{\pm ikr+g(r)}}{r}$$

$$\frac{d^2g}{dr^2}+\left(\frac{dg}{dr}\right)^2\pm 2ik\frac{dg}{dr}=\frac{2\gamma k}{r}$$

$$\pm i\frac{dg}{dr}=\frac{\gamma}{r}\quad\text{as}\quad r\to\infty$$

$$\psi(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}e^{-\pi\gamma/2}\Gamma(1+i\gamma)_1F_1(-i\gamma;1;i(kr-\mathbf{k}\cdot\mathbf{r}))$$

$${}_1F_1(a;b;w)=1+\tfrac{a}{b}w+\tfrac{a(a+1)}{b(b+1)}\tfrac{w^2}{2!}+\tfrac{a(a+1)(a+2)}{b(b+1)(b+2)}\tfrac{w^3}{3!}+\ldots$$

$$\psi(\mathbf{r})\sim e^{ikz+i\gamma\log(k(r-z))}-\underbrace{\frac{\gamma}{k(r-z)}\frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)}}_{f(\theta)/r}e^{ikr-i\gamma\log(k(r-z))}+\ldots$$

$$f(\theta)=-\frac{\gamma}{k}\frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)}\frac{r}{r-z}=-\frac{\gamma}{2k}\frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)}\frac{1}{\sin^2(\theta/2)}$$

$$\frac{d\sigma}{d\Omega}=|f(\theta)|^2=\left(\frac{mA}{2\hbar^2k^2}\right)^2\frac{1}{\sin^4(\theta/2)}$$

Recovering the Hydrogen Atom:
$\Gamma(z)$ has poles at $z=0,-1,-2,\ldots$, the scattering amplitude therefore has poles when

$$1+i\gamma=-(n-1)\quad\Rightarrow\quad k=-i\frac{mA}{\hbar^2}\frac{1}{n},\qquad n=1,2,3,\ldots$$

(???)

$$E_n=\frac{\hbar^2k^2}{2m}=-\frac{mA^2}{2\hbar^2}\frac{1}{n^2}$$

Coulomb scattering by LL3.136

(тут большие формулы, в теории лучше сперва напишу их!)

$$\psi=\left[1+\frac{1}{ik^3r(1-\cos\theta)}\right]\exp\left\{ikz+\frac{i}{k}\ln[kr(1-\cos\theta)]\right\}+$$
$$+\frac{f(\theta)}{r}\exp\left\{ikr-\frac{i}{k}\ln(2kr)\right\}$$

$f(\theta)=-\frac{1}{2k^2\sin^2(\theta/2)}\frac{\Gamma(1+i/k)}{\Gamma(1-i/k)}\exp\left(-\frac{2i}{k}\ln\sin\frac{\theta}{2}\right)$

$$\exp\left(2i\delta_l^{\text{Кул}}\right)\frac{\Gamma(l+1+i/k)}{\Gamma(l+1-i/k)}$$

$$f(\theta)=\frac{1}{2ik}\sum_l(2l+1)\frac{\Gamma(l+1+i/k)}{\Gamma(l+1-i/k)}P_l(\cos\theta)$$

$$\psi_{\mathbf{k}}^{(+)} = \frac{1}{2k}\sum_{l=0}^{\infty} i^l(2l+1)e^{i\delta_l}R_{kl}(r)P_l\left(\frac{\mathbf{rk}}{kr}\right)$$

$$\psi_{\mathbf{k}}^{(-)} = \psi_{-\mathbf{k}}^{(+)}$$

Для кулонова поля отталкивания:

$$\psi_{\mathbf{k}}^{(+)} = e^{-\pi/2k}\Gamma\left(1+\frac{i}{k}\right)e^{i\mathbf{kr}}F\left(-\frac{i}{k},1,i(kr-\mathbf{kr})\right)$$
$$\psi_{\mathbf{k}}^{(-)} = e^{-\pi/2k}\Gamma\left(1-\frac{i}{k}\right)e^{i\mathbf{kr}}F\left(\frac{i}{k},1,-i(kr+\mathbf{kr})\right)$$

Для поля притяжения получаются: замена знака у k и r:

$$\psi_{\mathbf{k}}^{(+)} = e^{\pi/2k}\Gamma\left(1-\frac{i}{k}\right)e^{i\mathbf{kr}}F\left(\frac{i}{k},i(kr-\mathbf{kr})\right)$$
$$\psi_{\mathbf{k}}^{(-)} = e^{\pi/2k}\Gamma\left(1+\frac{i}{k}\right)e^{i\mathbf{kr}}F\left(-\frac{i}{k},1,-i(kr+\mathbf{kr})\right)$$

Special useful methods for scattering

Слабо связанное состояние в мелкой яме через диаграммы для амплитуды рассеяния заменой на дельта-потенциал

Мелкая яма - яма у которой $U_0 \ll \hbar^2/2ma^2$, a - радиус ямы. Размер связанного состояния в такой яме много больше ее радиуса, а энергия связи - много меньше глубины ямы U_0.

В $D = 1$ заменим потенциал на δ-функцию $V(x) = -U_0a\delta(x)$, получаем фурье-компоненту $V(q) = -U_0a = \text{const}$, считаем:

$$F(k,k') = -U_0a + U_0a\int \frac{F(k,q)}{\varepsilon - q^2/2m + i\delta}\frac{dq}{2\pi}.$$

(?? поч?)

$$F(k) = -U_0a - \frac{U_0a}{2\pi}F(k)\int\limits_{-\infty}^{+\infty}\frac{2mdq}{q^2-k^2-i\delta},$$

$$\text{res} \Rightarrow \qquad F^{-1} + (U_0a)^{-1} = -im/k \equiv -i\sqrt{m/2\varepsilon}, \qquad \varepsilon := k^2/(2m)$$

$$F(\varepsilon) = -\frac{U_0a\sqrt{2(\varepsilon+i\delta)/m}}{\sqrt{2(\varepsilon+i\delta)/m}+iU_0a}.$$

Имеем полюс при $\varepsilon_0 = -mU_0^2a^2/(2\hbar^2)$, это известный уровень 1D δ-ямы.

For 2D well we compute by a cut-off: $V(k) = -U_0a^2$,

$$F(\varepsilon) = -U_0a^2 + U_0a^2\frac{2m}{\hbar^2}\int F(\varepsilon)\frac{2\pi q}{q^2-k^2-i\delta}\frac{dq}{(2\pi)^2},$$

Интеграл $\int\limits_0^\infty \frac{dq^2}{q^2-k^2-i\delta}$ логарифмически расходится на ∞, но при $q \geqslant a^{-1}$ фурье-компонента $V(k)$ начинает быстро осциллировать (??? какая она??), и интеграл с $V(k)$ сходится. Обрежем "вручную" при $q \approx a^{-1}$:

$$\int\limits_0^{a^{-2}} \frac{dq^2}{q^2-k^2-i\delta} = \pi i + \ln \frac{1}{a^2\left(k^2+i\delta\right)}$$

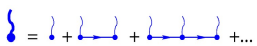
$$F(\varepsilon) \approx -\frac{U_0 a^2}{1+\left(2ma^2U_0/4\pi\hbar^2\right)\ln\left(-k^2a^2\right)} = -\frac{U_0 a^2}{1+\left(mU_0a^2/2\pi\hbar^2\right)\ln\left(-\varepsilon ma^2/\hbar^2\right)}$$

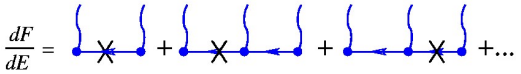
$$\varepsilon_0 \approx -\frac{\hbar^2}{ma^2}\exp\left(-\frac{2\pi\hbar^2}{ma^2U_0}\right)$$

Из-за неизвестного множителя порядка единицы, появившегося при обрезании перед логарифмом, ε_0 найден только по порядку величины.

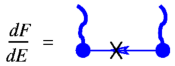
В $D > 2$ интеграл $\int\limits_0^{a^{-1}} \frac{q^{D-1}dq}{q^2-k^2-i\delta}$ остается конечным при $k \to 0$, поэтому для слабого потенциала $F(\varepsilon)$ не имеет полюсов при $|k| \ll a^{-1}$, т.е. нет связанного состояния.

Двумерное рассеяние методом логарифма и ренормгруппы

Дифференцируем  , (???)



$:= \frac{\partial}{\partial\varepsilon}G_0 = -\frac{1}{(\varepsilon-p^2/2m+i\delta)^2} = -G_0^2.$



$$\frac{\partial}{\partial\varepsilon}F_\varepsilon\left(k_1,k_2\right) = -\int \frac{F_\varepsilon\left(k_1,q\right)F_\varepsilon\left(q,k_2\right)}{\left(\varepsilon-q^2/2m+i\delta\right)^2}\frac{d^2q}{(2\pi)^2}$$

$F_\varepsilon\left(k_1,k_2\right)$ от k_1 и k_2 имеет характерный масштаб $k_{1,2} \approx a^{-1}$, поэтому при малых $|\varepsilon| \ll \varepsilon_a = \hbar^2/\left(ma^2\right)$ интеграл по q сходится в области, где зависимость F от q несущественна. Вычисляя интеграл (???), получаем

$$\frac{\partial}{\partial\varepsilon}F = -\frac{m}{2\pi\hbar^2\varepsilon}F^2.$$

$$F(\varepsilon) = \frac{2\pi\hbar^2}{m\ln\left((\varepsilon+i\delta)/\varepsilon_0\right)},$$

ε_0 - неизвестная константа. Точка ветвления логарифма при $\varepsilon = 0$ смещена в нижнюю полуплоскость. Константа ε_0 вещественна и отрицательна, поскольку при $\varepsilon < 0$ амплитуда F вещественна.

В итоге длня ε_0 в низкоэнергетической области, $|\varepsilon_0| \leqslant \varepsilon_a$, и полюс при $\varepsilon = \varepsilon_0$ имеет реальный смысл, ему соответствует дискретный уровень. В случае больших энергий полюс находится вне области энергий, где применимо сделанное приближение, и поэтому смысла не имеет.

On rigorous scattering theory

(пока не актуально, потом, может, изучу и создам пару разделов про это, очень много теории про неё.)

Об S матрице (!!!!!!!)

(главные ее свойства! супер важный параграф)

Математические свойства

В предыдущем разделе было показано, что для потенциалов $V(x)$, удовлетворяющих условию (2.2), операторы $H = H_0 + V$ и H_0 имеют один и тот же абсолютно непрерывный спектр. Среди множества операторов частичной изометрии в $\mathscr{H}$, устанавливающих унитарную эквивалентность между $H|_{\mathscr{H}_{\text{ac}}}$ и H_0, имеются два оператора $W_{\pm}$фундаментальной физической значимости. Они определяются как

$$W_{\pm} = \lim_{t \to \pm\infty} e^{iHt} e^{-itH_0}$$

где предел понимается в сильной операторной топологии, и называются волновыми операторами (или операторами Меллера). В общем случае волновые операторы существуют для оператора Шрёдингера $H = H_0 + V$ на $\mathbb{R}^n$ с потенциалом $V(\boldsymbol{q})$, достаточно быстро затухающим при $|\boldsymbol{q}| \to \infty$.

Для потенциалов $V(x)$, удовлетворяющих условию (2.2), пределы (2.31) существуют.

Волновые операторы используются для описания рассеяния квантовой частицы на потенциальном центре. А именно: для заданного $\varphi_- \in \mathscr{H}$, существует $\psi = W_-\varphi_- \in \mathscr{H}$, такое, что решение $\psi(t) = U(t)\psi$ нестационарного уравнения Шрёдингера с гамильтонианом H и начальным условием $\psi(0) = \psi$ при $t \to -\infty$ приближается к решению $\varphi_-(t) = U_0(t)\varphi_-$ нестационарного уравнения Шрёдингера со свободным гамильтонианом H_0 и начальным условием $\varphi_-(0) = \varphi_-$. Поскольку $\operatorname{Im} W_- = \operatorname{In} W_+$, существует $\varphi_+ \in \mathscr{H}$, такое, что $\psi = W_+\varphi_+$и решение $\psi(t)$ нестационарного уравнения Шрёдингера с гамильтонианом H и начальным условием $\psi(0) = \psi$ при $t \to \infty$ приближается к решению $\varphi_+(t) = U_0(t)\varphi_+$нестационарного уравнения Шрёдингера со свободным гамильтонианом H_0 и начальным условием $\varphi_+(0) = \varphi_+$. Переход от решения $\varphi_-(t)$ свободного уравнения Шрёдингера, описывающего движение квантовой частицы при $t = -\infty$, к решению $\varphi_+(t)$, описывающему ее движение при $t = \infty$, - результат рассеяния квантовой частицы потенциальным центром. Вся информация о рассеянии содержится в операторе рассеяния S (в физике также называемом S-матрицей), связывающем начальное и конечное условия φ_-и φ_+:

$$\varphi_+ = S\varphi_-.$$

Из (2.32) и $\psi = W_-\varphi_- = W_+\varphi_+$мгновенно получается, что

$$S = W_+^* W_-,$$

а из (2.32) - (2.34) получается, что оператор рассеяния S унитарен в $\mathscr{H}$ и коммутирует со свободным гамильтонианом H_0:

$$S^*S = SS^* = I \quad \text{и} \quad SH_0 = H_0S.$$

Это - набросок нестационарного подхода к теории рассеяния. В стационарном подходе к теории рассеяния волновые операторы $W_{\pm}$ и оператор рассеяния S строятся как

интегральные операторы в координатном представлении с интегральными ядрами, выраженными через особые решения стационарного уравнения Шрёдингера. Здесь мы представим эту конструкцию для одномерного оператора Шрёдингера, рассмотренного в предыдущем разделе.

$$S(k) = \begin{pmatrix} s_{11}(k) & s_{12}(k) \\ s_{21}(k) & s_{22}(k) \end{pmatrix}$$

называется матрицей рассеяния. Из (2.14) следует, что матрица рассеяния унитарна, $S^*(k)S(k) = I$, где I - единичная матрица 2×2, и удовлетворяет условию $\overline{S(k)} = S(-k)$. В частности, из унитарности матрицы рассеяния следует, что $T + R = 1$, что называется сохранением вероятности.

(???? хз????)

Имеется эквивалентность стационарного и нестационарного подходов к теории рассеяния:

Теорема 2.5. Для одномерного оператора Шрёдингера $H = H_0 + V$ с потенциалом $V(x)$, удовлетворяючии условию (2.2), волновые операторы существуют и могут быть заданы явными формулами

$$W_\pm = \mathscr{U}_\pm^* \mathscr{U}_0,$$

где $\mathscr{U}_\pm : \mathscr{H} \to \mathfrak{H}_0$ - интегральные операторы, задаваемые формулами

$$\mathscr{U}_\pm(\psi) = \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} \psi(x) \overline{U_\pm(x, \sqrt{\lambda})} dx$$

а оператором $\mathscr{U}_0 : \mathscr{H} \to \mathfrak{H}_0$ устанавливается унитарная эквивалентность между оператором H_0 в $\mathscr{H}$ и оператором умножения на λ в $\mathfrak{H}_0$,

$$\mathscr{U}_0(\psi) = \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} \psi(x) \begin{pmatrix} e^{-i\sqrt{\lambda}x} \\ e^{i\sqrt{\lambda}x} \end{pmatrix} dx.$$

Оператор рассеяния S в $\mathscr{H}$ и оператор умножения на матрицу рассеяния $S(\sqrt{\lambda})$ на $\mathfrak{H}_0$ унитарно эквивалентны:

$$S = \mathscr{U}_0^* S(\sqrt{\lambda}) \mathscr{U}_0.$$

Следствие 2.6. Волновые операторы удовлетворяют соотношениям ортогональности и полноты $W_\pm^* W_\pm = I$ и $W_\pm W_\pm^* = I - P$.

Уравннеие Липпмана-Швингера и операторы по Тахтаджаяну (???)

В терминах операторов $\mathscr{U}_\pm : \mathscr{H} \to \mathscr{H}$, $\mathscr{U}_\pm(\psi)(\boldsymbol{k}) := (2\pi)^{-\frac{3}{2}} \int\limits_{\mathbb{R}^3} \psi(\boldsymbol{x}) u^{(\pm)}(\boldsymbol{x}, \boldsymbol{k}) d^3\boldsymbol{x}$, соотношения полноты и ортогональности принимают вид

$$\mathscr{U}_\pm^* \mathscr{U}_\pm = I - P, \quad \mathscr{U}_\pm \mathscr{U}_\pm^* = I,$$

где P - ортогональная проекция на инвариантное подпространство для оператора H, ассоциированное с чисто точечным спектром. Теперь пусть

$$W_\pm = \mathscr{U}_\pm^* \mathscr{U}_0$$

где $\mathscr{U}_0 = \mathscr{F}^{-1}$ - обратное преобразование Фурье.

(???? дочитаю!)

О других граничных условиях (????)

Предположим, что потенциал $V(x)$ удовлетворяет условию

$$\int\limits_{-\infty}^{0}(1+|x|)\left|V(x)-c^2\right|dx<\infty \quad \text{и} \quad \int\limits_{0}^{\infty}(1+|x|)|V(x)|dx<\infty$$

Абсолютно непрерывный спектр оператора Шрёдингера H заполняет $[0,\infty)$. При $0<\lambda=k^2<c^2$ спектр прост, а

$$u(x,\lambda)=\frac{1}{a(k)}f_2(x,k), \quad 0<k<c,$$

- это аналоги нормированных собственных функций непрерывного спектра. При $\lambda=k^2>c^2$ спектр имеет кратность два, и

$$u_1(x,\lambda)=\frac{1}{a(k)}f_2(x,k), \quad u_2(x,k)=\frac{k_1}{ka(k)}f_1(x,k), \quad k>c,$$

- это аналоги нормированных собственных функций непрерывного спектра.

Допустим, что потенциал $V(x)$ растет при $x\to-\infty$ и затухает при $x\to\infty$:

$$\int\limits_{a}^{\infty}(1+|x|)|V(x)|dx<\infty \qquad \forall a,$$

и что существует $x_0\in\mathbb{R}$, такое, что спектр задачи Штурма - Лиувилля

$$-y''+V(x)y=\lambda y, \quad -\infty<x\leqslant x_0, \quad \text{и} \quad y'(x_0)=0$$

ограничен снизу и дискретен. Последнее условие - это конкретная формулировка свойства $\lim_{x\to-\infty}V(x)=\infty$.

Тогда для любого вещественного k существует решение $f(x,k)$ дифференциального уравнения (2.43) с асимптотикой

$$f(x,k)=e^{ikx}+o(1) \quad \text{при} \quad x\to\infty$$

и существует функция $s(k)$, такая, что

$$u(x,k)=f(x,-k)+s(k)f(x,k)$$

интегрируемо с квадратом на промежутке $(-\infty,a)$ для любого вещественного a. Оператор Шрёдингера H имеет простой абсолютно непрерывный спектр $[0,\infty)$ и дискретный спектр, состоящий из конечного числа отрицательных собственных значений.

21.1.5 Details of typical QM methods for simple atoms

(там ЛЛ3, много всякого есть, что хочется сказать, но точно не нужно знать в рамках минимального понимания атомов)

Другие общие свойства атома водорода

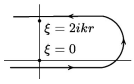
Вывод непрерывного спектра в центральном поле в сферических координатах

(!?!?!?? это сесть и продумать заново нужно!!!)

$$n = -\frac{i}{\sqrt{2E}} = -\frac{i}{k}, \quad \rho = 2ikr$$

$$R_{kl} = \frac{C_{kl}}{(2l+1)!}(2kr)^l e^{-ikr} F\left(\frac{i}{k} + l + 1, 2l+2, 2ikr\right),$$

$$R_{kl} = C_{kl}(2kr)^l e^{-ikr} \cdot \frac{1}{2\pi i} \oint e^{\xi} \left(1 - \frac{2ikr}{\xi}\right)^{-\frac{i}{k}-l-1} \xi^{-2l-2} d\xi$$



$$\xi \equiv 2ikr(t + 1/2)$$

$$R_{kl} = C_{kl}\frac{(-2kr)^{-l-1}}{2\pi} \oint e^{2ikrt} \left(t + \frac{1}{2}\right)^{\frac{i}{k}-l-1} \left(t - \frac{1}{2}\right)^{-\frac{i}{k}-l-1} dt$$

$$\approx \frac{2}{r} \sin\left(kr + \frac{1}{k}\ln 2kr - \frac{\pi}{2}l + \delta_l\right),$$

$$\delta_l = \arg\Gamma\left(l + 1 - \frac{i}{k}\right)$$

$$C_{kl} = \left[\frac{8\pi k}{1 - e^{-2\pi/k}}\right]^{1/2} \prod_{s=1}^{l} \sqrt{s^2 + \frac{1}{k^2}}$$

(словами напишу, что за математика тут)

Водород в параболических координатах по ЛЛ3.37

(тут суть и преимущества)

Каждое стационарное состояние дискретного спектра определяется в параболических координатах «тремя целыми параболическими квантовыми числами» n_1 и n_2 и m. Для числа n («главное квантовое число») имеем из (37.9) и (37.12)

$$n = n_1 + n_2 + |m| + 1.$$

Для уровней энергии получается, разумеется, прежний результат (36.9).

При заданном n число $|m|$ пробегает n значений от 0 до $n-1$. При фиксированных n и $|m|$ число n_1 пробегает $n - |m|$ значений от 0 до $n - |m| - 1$; также при заданном $|m|$ можно еще выбрать функции с $m = \pm|m|$, поэтому всего для данного n имеется уровней (???)

$$2\sum_{m=1}^{n-1}(n-m) + (n-0) = n^2$$

$$x = \sqrt{\xi\eta}\cos\varphi, \quad y = \sqrt{\xi\eta}\sin\varphi, \quad z = \frac{1}{2}(\xi - \eta),$$

$$r = \sqrt{x^2 + y^2 + z^2} = \frac{1}{2}(\xi + \eta)$$

$$\xi = r + z, \quad \eta = r - z, \quad \varphi = \operatorname{arctg}\frac{y}{x};$$

$$dl^2 = \frac{\xi+\eta}{4\xi}d\xi^2 + \frac{\xi+\eta}{4\eta}d\eta^2 + \xi\eta d\varphi^2, \qquad dV = \frac{1}{4}(\xi+\eta)d\xi d\eta d\varphi.$$

$$\Delta = \frac{4}{\xi+\eta}\left[\frac{\partial}{\partial\xi}\left(\xi\frac{\partial}{\partial\xi}\right) + \frac{\partial}{\partial\eta}\left(\eta\frac{\partial}{\partial\eta}\right)\right] + \frac{1}{\xi\eta}\frac{\partial^2}{\partial\varphi^2}.$$

$$\int |\psi_{n_1n_2m}|^2\, dV = \tfrac{1}{4}\int_0^\infty\int_0^\infty\int_0^{2\pi} |\psi_{n_1n_2m}|^2\,(\xi+\eta)d\varphi d\xi d\eta \equiv 1,$$

$$\psi_{n_1n_2m} = \frac{\sqrt{2}}{n^2} f_{n_1m}\left(\frac{\xi}{n}\right) f_{n_2m}\left(\frac{\eta}{n}\right)\frac{e^{im\varphi}}{\sqrt{2\pi}}$$

$$f_{pm}(\rho) := \frac{1}{|m|!}\sqrt{\frac{(p+|m|)!}{p!}}F(-p,|m|+1,\rho)e^{-\rho/2}\rho^{|m|/2}.$$

Волновые функции в параболических координатах, в противоположность волновым функциям в сферических координатах, не симметричны относительно плоскости $z=0$. При $n_1 > n_2$ вероятность нахождения частицы на стороне $z>0$ больше, чем на стороне $z<0$, а при $n_1 < n_2$ - наоборот (??? додумаю??).

(где используется это вообще???)

Поляризуемость атома водорода в основном состоянии

(см. ЛЛ3 стр 354, задача есть на это, укажу на 1/4 страницы идею и основные формулы, а то не очевидно)

О других применениях модели водорода

(буду узнавать - буду дописывать)

О падении на центр по ЛЛ3 пар 35 (??)

$$R'' + \frac{2}{r}R' + \frac{\gamma}{r^2}R = 0 \qquad \gamma := \frac{2m\beta}{\hbar^2} - l(l+1)$$

(тут словами переходы укажу)

$$R = \text{ const } \cdot \frac{1}{\sqrt{r}}\cos\left(\sqrt{\gamma - \frac{1}{4}}\ln\frac{r}{r_0} + \text{ const }\right).$$

«Критическое» поле $U_{\text{кр}}$, при котором становится возможным падение частицы на центр, соответствует значению $\gamma = 1/4$. Наименьшее значение коэффициента при $-1/r^2$ получается, когда $l=0$, т. е.

$$U_{\text{кр}} = -\frac{\hbar^2}{8mr^2}$$

(тут еще качественный анализ, додумаю его!)

Дискретный спектр в центральном поле в сферических координатах

(суть ЛЛ3 пар 36. не понял пока, что тут особенного???)

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{l(l+1)}{r^2}R + \frac{2m}{\hbar^2}\left(E + \frac{\alpha}{r}\right)R = 0$$

$$\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}-\frac{l(l+1)}{r^2}R+2\left(E+\frac{1}{r}\right)R=0$$

$$n:=\frac{1}{\sqrt{-2E}},\quad \rho:=\frac{2r}{n}$$

$$E=-\frac{m\alpha^2}{2\hbar^2n^2}$$

Волновые функции стационарных состояний определяются формулами (36.5), (36.7).

Вырожденная гипергеометрическая функция с целыми значениями обоих параметров совпадает с обобщенными полиномами Лагерра (с точностью до множителя):

$$R_{nl}=\ \text{const}\ \cdot\rho^l e^{-\rho/2}L_{n+1}^{2l+1}(\rho).$$

$\int\limits_0^\infty R_{nl}^2r^2dr=1.$

$$R_{nl}=-\frac{2}{n^2}\sqrt{\frac{(n-l-1)!}{[(n+l)!]^3}}e^{-r/n}\left(\frac{2r}{n}\right)^l L_{n+l}^{2l+1}\left(\frac{2r}{n}\right)=$$

$$=\frac{2}{n^{l+2}(2l+1)!}\sqrt{\frac{(n+l)!}{(n-l-1)!}}(2r)^l e^{-r/n}F\left(-n+l+1,2l+2,\frac{2r}{n}\right)$$

21.2 Typical numerical methods

21.2.1 On density functional theory

(нужно будет - изучу, готов уже)

Basic theory of DFT

Hohenberg-Kohn theorem

Kohn-Sham equations

The transformation of the Hohenberg-Kohn theorem from a curiosity into a useful tool takes place via the Kohn-Sham (KS) approach and via a simple approximation known as Local-Density Approximation, LDA (1965). Since the Hohenberg-Kohn theorem holds irrespective of the electron-electron repulsion U, we may introduce an auxiliary system of non-interacting electrons having the same density as the true system:

$$\rho(\mathbf{r})=\sum_i|\psi_i(\mathbf{r})|^2$$

where the ψ_i (Kohn-Sham orbitals) are single-electron wavefunctions, to be determined by the condition that $E[\rho]$ is minimized, under orthonormality constraints $\langle\psi_i|\psi_j\rangle=\delta_{ij}$. We still do not know the functional to be minimized, but let us write it as a sum of known terms, large and easy to compute, and the rest:

$$E=T_s[\rho]+E_H[\rho]+\int\rho(\mathbf{r})v(\mathbf{r})d^3r+E_{xc}[\rho]$$

where T_s is the kinetic energy of the non-interacting electrons:

$$T_s = -\frac{\hbar^2}{2m}\sum_i \int \psi_i^*(\mathbf{r})\nabla^2\psi_i(\mathbf{r})d^3r$$

(note that in general $T_s \neq \langle\Psi|T|\Psi\rangle$), E_H is the electrostatic (Hartree) energy:

$$E_H[\rho] = \frac{q_e^2}{2}\int \frac{\rho(\mathbf{r})\rho\left(\mathbf{r}'\right)}{|\mathbf{r}-\mathbf{r}'|}d^3r d^3r'$$

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V_{KS}(\mathbf{r})\right)\psi_i(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r})$$

where the effective, or Kohn-Sham potential, $V_{KS} = v(\mathbf{r}) + V_H(\mathbf{r}) + V_{xc}(\mathbf{r})$, is a functional of the charge density:

$$V_H(\mathbf{r}) = q_e^2\int \frac{\rho\left(\mathbf{r}'\right)}{|\mathbf{r}-\mathbf{r}'|}d^3r', \quad V_{xc}(\mathbf{r}) = \frac{\delta E_{xc}[\rho]}{\delta\rho(\mathbf{r})}$$

KS equations are reminiscent of Hartree-Fock equations, Eq.(6.19), with the exchange potential replaced by the exchange-correlation potential. Note that the latter is a local potential, while the exchange potential is non-local. The energy can be rewritten using the sum over KS eigenvalues ϵ_i. It is straightforward to prove that the energy functional can be written as

$$E = \sum_i \epsilon_i - E_H[\rho] + E_{xc} - \int \rho(\mathbf{r})V_{xc}(\mathbf{r})d^3r$$

Approximated functionals

Not much progress seems to be done yet: E_{xc} is still an unknown functional, and so is V_{xc}. There is however a long tradition, pre-dating DFT, of using homogeneous electron gas results to approximate similar functions. The most famous historical method is Slater's local approximation to the exchange potential:

$$V_x(\mathbf{r}) \simeq -\frac{3q_e^2}{2\pi}\left(3\pi^2\rho(\mathbf{r})\right)^{(1/3)}$$

Kohn and Sham extend and improve upon such ideas by introducing the local density approximation (LDA): they re-write the the energy functional as

$$E_{xc} = \int \rho(\mathbf{r})e_{xc}(\mathbf{r})d^3r$$

Structure of a DFT code

The basic [3] algorithm for the solution of the DFT problem consists of a self-consistent loop in which, at iteration n:

1. the KS potential $V_{KS}^{(n)}$ is computed from $\rho^{(n)}$.
2. KS equations are solved, yielding KS orbitals $\psi_i^{(n)}$;
3. the output charge density $\rho_{\text{out}}^{(n)}$ is calculated by summing the square of all occupied KS orbitals: $\rho_{\text{out}}^{(n)} = \sum_i \left|\psi_i^{(n)}\right|^2$;
4. the new charge density $\rho^{(n+1)}$ is computed from a linear combination of previous input $\rho^{(n)}$ and output $\rho_{\text{out}}^{(n)}$ charge densities.

(see lectures by Paolo Giannozzi)

Time-dependent density functional theory (????)

Thomas–Fermi model (????)

Orbital-free density functional theory (????)

Linearized augmented-plane-wave method (????)

Projector augmented wave method (????)

21.2.2 Typical modeling in Wolfram

(см. книгу Schmiedt-a, впишу основные коды сюда!)

21.3 Fundamentals of QM: details

21.3.1 Open quantum systems: formalism

(see a special note about it for now)

О матрице плотности (!?!??!??!)

(пересмотрю Филиппова потом, дополню им этот раздел! важный раздел для приложений!!!)

Суть

$$\langle \hat{O} \rangle = \sum_{\alpha} p_\alpha \langle \alpha | \hat{O} | \alpha \rangle = \mathrm{Tr}\left(|\alpha\rangle p_\alpha \langle \alpha | \hat{O} \right) \equiv \mathrm{Tr}(\hat{\rho}\hat{O}),$$

$$\hat{\rho} = \sum_{\alpha} p_\alpha |\alpha\rangle\langle\alpha|$$

$$\bar{f} = \int \left[\hat{f} \rho\left(x, x'\right) \right]_{x'=x} dx$$

(????)

$$\rho\left(x, x'\right) = \int \Psi(q, x) \Psi^*\left(q, x'\right) dq$$

Матрица плотности имеет свойства:
$\rho^*\left(x, x'\right) = \rho\left(x', x\right)$.

$$\mathrm{Tr}\,\hat{\rho} = \sum_{\alpha\beta} \psi_{\alpha\beta} \psi^*_{\alpha\beta} = 1$$

положительно определенность

$$\frac{\partial \hat{\rho}}{\partial t} = \frac{i}{\hbar} [\hat{\rho}(t), \hat{H}]$$

Введя этот объект мы видим, что из него можно с помощью *частичного следа* получать объект, описывающий подсистемы:

$$\hat{\rho}_A = \mathrm{Tr}_B\, \hat{\rho}_{AB} \leftrightarrow \left(\hat{\rho}_A\right)_{\alpha\alpha'} = \sum_{\beta} \left(\hat{\rho}_{AB}\right)_{\alpha\beta,\alpha'\beta}$$

как кстати обратно к волновой функции прийти?
на практике мы используем

$$\hat{\rho} = \sum_n p_n |n\rangle\langle n|, \quad 0 \le p_n \le 1, \quad \sum_n p_n = 1$$

Для любых двухуровневых систем она имеет такой вид: $\hat{\rho} = \frac{1}{2}(\hat{\mathbb{I}} + \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n})$

Пусть $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, занумеруем базисные элементы $\{|\alpha\rangle\} \in \mathcal{H}_A$ и $\{|\beta\rangle\} \in \mathcal{H}_B$, преобразуем наблюдаемую величину для системы A оператор дает δ-функцию и в итоге мы приходим к этим переходам.

(потом еще подумаю про это):

$$\langle\psi_{AB}|\hat{O}_A|\psi_{AB}\rangle = \sum_{\alpha\beta,\alpha'\beta'} \langle\psi_{AB}|\alpha'_A,\beta'_B\rangle \left\langle \alpha'_A,\beta'_B \left| \hat{O}_A \right| \alpha_A,\beta_B \right\rangle \langle\alpha_A,\beta_B|\psi_{AB}\rangle =$$
$$= \sum_{\alpha\alpha'} \underbrace{\sum_{\beta} \psi_{\alpha\beta}\psi_{\alpha^*\beta}}_{\equiv(\hat{\rho}_A)_{\alpha\alpha'}} \left(\hat{O}_A\right)_{\alpha'\alpha} \equiv \mathrm{Tr}(\hat{\rho}_A\hat{O}_A)$$

Тут $(\hat{\rho}_A)_{\alpha\alpha'} = \sum_\beta \psi_{\alpha\beta}\psi^*_{\alpha'\beta}$

появление матрицы плотности

как конкретно она появляется?

Другое важное о матрице плотности

(там много очень всего, так что точно что-то еще полезно будет указать.)

9.3

Модель Калдейры – Леггетта

(см. пока лекции ПТФ, просто не нужно это было, нет возможности вписывать это сейчас.)

9.3.1

Приближение Борна – Маркова

. 109 9.3.2

Операторный формализм

110 9.3.3

Спектральный вес и омическая баня

dissipative evolutions,

decoherence,

Caldeira-Leggett model.

Weak coupling (Fermi-Golden rule),

Lindblad equation;

21.3.2 Parameters for constructing models

Typical parameters

$$\phi(\mathbf{r}) = \frac{q}{r} + \frac{\mathbf{d}\cdot\mathbf{r}}{r^3} + \frac{1}{6}\sum_{ij}\frac{Q_{ij}T_{ij}}{r^5} + ..., \quad T_{ij} = 3x_ix_j - r^2\delta_{ij}$$

$$q = \int d\mathbf{r}\rho(\mathbf{r}), \quad \mathbf{d} = \int d\mathbf{r}\rho(\mathbf{r})\mathbf{r}, \quad Q_{ij} = \int d\mathbf{r}\rho(\mathbf{r})T_{ij}$$

$$\mathbf{A}(\mathbf{r}) = \frac{\boldsymbol{\mu}\times\mathbf{r}}{r^3}, \quad \boldsymbol{\mu} = \frac{1}{2}\int d\mathbf{r}\mathbf{r}\times\mathbf{J}(\mathbf{r})$$

(потом напишу, там много особенностей ее)

(потом напишу, там много особенностей его, в КТП еще подробнее про него, тут лишь результаты напишу)

(тут только +- общефиз, а также типичный квантмех про это)

21.3.3 The Meaning and Main Interpretations of Quantum Mechanics (???)

(пока этим не занимаюсь, это очень большие вопросы, при этом многое можно сделать, абсолютно плохо это понимая.)

В чем же суть квантовой механики?

(потом пропишу свой ответ)

Что такое квантовые флуктуации?

(они мб важные, но пока так я и мало въехал в них)

О казуальной неопределенности (??)

и все про неопределенность и ее влияние на все

казуальная - просто умное слово, по факту типичная неубираемая неопределенность, которая нам уже известна.

Откуда могут быть вообще потенциалы и стенки (???)

Если частица описывается волновой функцией, то как может быть так, что есть какой-то центр, который создает центральный потенциал? как может быть стенка? ведь там же тоже частицы, которые тоже описываются волновой функцией.

Как по волновой функции восстановить потенциал?

Как на квантовом уровне устроен мир?

(потом пропишу свой ответ)

О переходе от частицам к волнам (!??!??!?!?!?!)

(потом пропишу свой ответ. Пока отвечаю на это в рамках типичной квантовой теории поля, и такой ответ мне совершенно не нравится.)

наглядный переход от частицы к волне

снова этим же вопросом задамся и найду ответ.
???

О квантовых полях и квантовой механике (???)

О связи квантовой механики и классической

О функционале достоверности Киселева (??)

(?? пока только тут про него, скоро допишу!!!)

О переходе в классику усреднением, теореме вириала, теореме Эренфеста

(???? подумаю про это позже еще??? пока для меня это просто общие свойства, ничего применяющегося. так что потом это додумаю.)

По теореме Эренфеста динамика средней величины имеет вид:

$$\frac{d}{dt}\langle A\rangle = \frac{1}{i\hbar}\langle [A,H]\rangle + \left\langle \frac{\partial A}{\partial t}\right\rangle$$

В частности:

$$\frac{d}{dt}\langle q\rangle = \frac{1}{m}\langle p\rangle$$
$$\frac{d}{dt}\langle p\rangle = -\left\langle \frac{\partial U}{\partial q}\right\rangle$$

Квантовая *теорема вириала*:

$$-2\langle \hat{T}\rangle + \left\langle \boldsymbol{r}\frac{\partial V}{\partial \boldsymbol{r}}\right\rangle = 0$$

(??? строчка обоснований!)

$$V(x)\sim x^{\nu} \qquad \Rightarrow \qquad 2\bar{T} = \nu\bar{V}.$$

Proof by Tong:
$V(\mathbf{x}) = Ar^n$
$V(\lambda\mathbf{x}) = \lambda^n V(\mathbf{x})$

$$E_0 = \int d^d\mathbf{x}\frac{\hbar^2}{2m}\left|\nabla\psi_0(\mathbf{x})\right|^2 + V(\mathbf{x})\left|\psi_0(\mathbf{x})\right|^2 \equiv \langle T\rangle_0 + \langle V\rangle_0$$

$\psi(\mathbf{x}) = \alpha^{d/2}\psi_0(\alpha\mathbf{x})$,

$$E(\alpha) = \alpha^2\langle T\rangle_0 + \alpha^{-n}\langle V\rangle_0$$

$$\frac{dE}{d\alpha} = 2\alpha\langle T\rangle_0 - n\alpha^{-n+1}\langle V\rangle_0 = 0$$

$\alpha = 1$

$$2\langle T\rangle_0 = n\langle V\rangle_0$$

О связи квантовой механики и КТП (????)

(пока тут, мб подподглаву создам потом)

21.3.4 Constants of quantum mechanics

fine structure constant $\frac{e^2}{\hbar c} = \alpha_{\text{em}}$

(?? experiments?)

Plank's constant

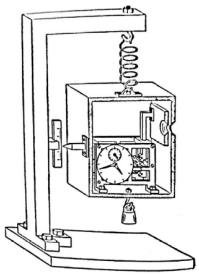
(?? experiments?)

21.3.5 Other important real and thought experiments

(I'll add them later, there are a lot of articles)

Einstein's light box

(см. нпр эксперименты Эйнштейна https://en.wikipedia.org/wiki/Einstein%27s_thought_experiments. потом разберу разные, напишу самые многое иллюстрирующие!)



On Einstain-Podolski-Roren thought experiment

(EPR, later I'll write)

21.3.6 Uncertainty Relation (????)

(в конце, потому что да, оно основное в квантмехе, но так прямо знать его не приходилось нужным.)

О соотношении неопределенностей

Основные формулы

Если наблюдаемая $A, B, C : [A, B] = i\hbar C$, то

$$\Delta A \Delta B \geq \frac{\hbar}{2}|\langle C \rangle|$$

В частности

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

(??? смысл выше формулы нужно пояснить!!!)
(!!! больше частных случаев???)
Доказывается соотношение неопределенностей из

$$(\Delta F)^2 := \langle \Psi | (\hat{F} - \overline{F})^2 | \Psi \rangle$$

$\overline{A} = \langle \psi | \hat{A} | \psi \rangle, \overline{B} = \langle \psi | \hat{B} | \psi \rangle$.

$$\hat{a} = \hat{A} - \overline{A}, \quad \hat{b} = \hat{B} - \overline{B}$$

Коммутатор операторов $[\hat{A}, \hat{B}] = i\hbar\hat{C}$ после сдвига не изменится:

$$[\hat{a}, \hat{b}] = i\hbar\hat{C}$$

Средние малых операторов по построению равны нулю: $\langle i|\hat{a}|i\rangle = 0, \langle i|\hat{b}|i\rangle = 0$, а дисперсия такая же, как и у больших.

$$|\Phi\rangle = (\hat{a} - i\xi\hat{b})|\Psi\rangle$$

Из $\langle \Psi | (\hat{a} - i\xi\hat{b})^\dagger (\hat{a} - i\xi\hat{b}) | \Psi \rangle \geq 0$ получаем:

$$\Delta A \Delta B \geq \frac{\hbar}{2}|\langle C \rangle|$$

Если у нас

$$[\hat{q}, \hat{p}] = i\hbar,$$

то имеем $\hat{C} = 1$, так что:

$$\Delta q \Delta p \geq \frac{\hbar}{2}$$

Обобщенное соотношение неопределенности Гейзенберга (Г. Вейль). Пусть $A, B \in \mathscr{A}$ и пусть $M = P_\psi$ - чистое состояние, такое, что $\psi \in D(A) \cap D(B) \boldsymbol{u} A\psi, B\psi \in D(A) \cap D(B)$. Тогда

$$\sigma_M^2(A)\sigma_M^2(B) \geqslant \frac{1}{4}\langle i[A, B]|M\rangle^2.$$

Такое же неравенство выполняется для любого $M \in \mathscr{S}$, где по определению $\langle i[A, B]||M\rangle = \lim_{n\to\infty} \langle i\left[A_n, B_n\right]|M\rangle$.

(строчка, как соотн неопр связано с УШ?)

(строчка, относится ли оно к измерениям или без измерений тоже оно как-то проявляется???)

(с ним столько проблем, что отдельный раздел сделал про него. вообще не понимаю его)

О применениях соотношения неопределенностей (!!!)

(очень часто оно применяется, тут укажу!!! под рукой всегда будет!!)

21.3.7 Other features of basics of QM

О функциях Йоста

(?? все то же самое, только называется сложно?)
Пусть

$$\sigma(x) = \int\limits_x^\infty |V(s)|ds \quad \text{и} \quad \sigma_1(x) = \int\limits_x^\infty \sigma(s)ds.$$

Поскольку $V \in L^1(\mathbb{R})$, имеем $\lim_{x\to\infty} \sigma(x) = 0$ и, используя условие (2.2) и теорему Фубини, получаем

$$\sigma_1(x) = \int\limits_x^\infty \int\limits_s^\infty |V(t)|dtds = \int\limits_x^\infty \int\limits_x^t |V(t)|dsdt = \int\limits_x^\infty (t-x)|V(t)|dt < \infty,$$

так что $\sigma \in L^1(x,\infty)$ для любого $x \in \mathbb{R}$ и $\lim_{x\to\infty} \sigma_1(x) = 0$. Аналогично функции

$$\tilde\sigma(x) = \int\limits_{-\infty}^x |V(s)|ds \quad \text{и} \quad \bar\sigma_1(x) = \int\limits_{-\infty}^x \bar\sigma(s)ds$$

удовлетворяют условию $\lim_{x\to-\infty} \tilde\sigma(x) = \lim_{x\to-\infty} \bar\sigma_1(x) = 0$. Условие (2.2) гарантирует, что для вещественных k дифференциальное уравнение (2.1) имеет решения $f_1(x,k)$ и $f_2(x,k)$, однозначно определяемые следующими асимптотиками:

$$\begin{aligned} f_1(x,k) &= e^{ikx} + o(1) \quad &&\text{при} \quad x \to \infty, \\ f_2(x,k) &= e^{-ikx} + o(1) \quad &&\text{при} \quad x \to -\infty. \end{aligned}$$

Они называются решенияии Йоста и играют фундаментальную роль в теории одномерного уравнения Шрёдингера.

Теорема 2.1. Для вечественных k дифференциальное уравнение (2.1) имеет решения $f_1(x,k)$ и $f_2(x,k)$, удовлетворяючие следующим свойствам.

(i) Оценки для $k \in \mathbb{R}$:

$$\begin{aligned} \left|e^{-ikx} f_1(x,k) - 1\right| &\leqslant \left(\sigma_1(x) - \sigma_1\left(x + \tfrac{1}{|k|}\right)\right) e^{\sigma_1(x)}, \\ \left|e^{ikx} f_2(x,k) - 1\right| &\leqslant \left(\tilde\sigma_1(x) - \tilde\sigma_1\left(x - \tfrac{1}{|k|}\right)\right) e^{\bar\sigma_1(x)}. \end{aligned}$$

(ii) Асимптотики при $|x| \to \infty$:

$$\begin{aligned} \lim_{x\to\infty} e^{-ikx} f_1(x,k) = 1, \quad \lim_{x\to\infty} e^{-ikx} f_1'(x,k) = ik, \\ \lim_{x\to-\infty} e^{ikx} f_2(x,k) = 1, \quad \lim_{x\to-\infty} e^{ikx} f_2'(x,k) = -ik. \end{aligned}$$

(iii) Аналитичность: функции $f_1(x,k)$ и $f_2(x,k)$ допускают аналитическое продолжение в верхнюю полуплоскость $\operatorname{Im} k > 0$ и являются непрерывными в области $\operatorname{Im} k \geqslant 0$ равномерно по x на компактных подмножествах $\mathbb{R}$.

(iv) Свойство сопряжения:

$$\overline{f_1(x,k)} = f_1(x,-\bar k), \quad \overline{f_2(x,k)} = f_2(x,-\bar k), \quad \operatorname{Im} k \geqslant 0.$$

(v) Оценки в части (i) выполняются для $\operatorname{Im} k \geqslant 0$. Для $k \neq 0$

$$\left|f_1(x,k) - e^{ikx}\right| \leqslant \frac{e^{-\operatorname{Im} kx}}{|k|}\sigma(x)e^{\frac{1}{|k|}\sigma(x)},$$
$$\left|f_2(x,k) - e^{-ikx}\right| \leqslant \frac{e^{\operatorname{Im} kx}}{|k|}\tilde{\sigma}(x)e^{\frac{1}{|k|}\tilde{\sigma}(x)}.$$

(vi) Асимптотика при $|k| \to \infty, \operatorname{Im} k \geqslant 0$:

$$e^{-ikx}f_1(x,k) = 1 + O\left(|k|^{-1}\right), \quad e^{ikx}f_2(x,k) = 1 + O\left(|k|^{-1}\right).$$

Следствие 2.2. Для $\operatorname{Im} k \geqslant 0 u k \neq 0$.

$$\lim_{x\to\infty} e^{-ikx}\left(\dot{f}_1(x,k) - ixf_1(x,k)\right) = 0, \quad \lim_{x\to-\infty} e^{ikx}\left(\dot{f}_2(x,k) + ixf_2(x,k)\right) = 0,$$

где точка обозначает частную производную по k.

Предложение 2.1. функчии $a(k)$ в верхней полуплоскости $\operatorname{Im} k > 0$ лишь конечное число чисто мнимых простых нулей $k_l = i\varkappa_l, \boldsymbol{u}$

$$\dot{a}\left(i\varkappa_l\right) = -ic_l \left\|f_2\left(\cdot, i\varkappa_l\right)\right\|^2, \quad l = 1, ..., n$$

где точка обозначает производную, $f_1\left(x, i\varkappa_l\right) = c_l f_2\left(x, i\varkappa_l\right)$. Функчия $1/a(k)$ ограничена в некоторой окрестности точки $k = 0$ в обласmu $\operatorname{Im} k \geqslant 0$.

Собственные значения оператора Шрёдингера H просты. Действительно, функция $f_1(x, i\varkappa)$ - решение дифференциального уравнения (2.1) для $\lambda = -\varkappa^2 < 0$, экспоненциально затухающее при $x \to \infty$. Поскольку вронскиан любых двух решений (2.1) постоянен, другое решение (2.1), линейно независимое с $f_1(x, i\varkappa)$, экспоненциально возрастает при $x \to \infty$. Таким образом, любое экспоненциально затухающее при $x \to \infty$ решение (2.1) для $\lambda = -\varkappa^2$ отличается от $f_1(x, i\varkappa)$ на постоянный множитель. В частности, это доказывает, что точечный спектр H прост. Этот результат следует также из простоты нулей функции $a(k)$ и теоремы о разложении по собственным функциям, которую мы докажем в следующем разделе.

О разложении по собственным функциям (????)

Построим ядро резольвенты для одномерного оператора Шрёдингера H и покажем, что оно самосопряжено и имеет область определения, состоящую из функций $\psi \in L^2(\mathbb{R})$, дважды дифференцируемых на $\mathbb{R}$ и таких, что $-\psi'' + V(x)\psi \in L^2(\mathbb{R})$. С помощью комплексного интегрирования мы выведем теорему о разложении собственных функций для оператора H, обобщающую соответсвующий результат для оператора H_0 свободной квантовой частицы, рассмотренный в разделе 2.2.3 главы 2.

Для $\lambda \in \mathbb{C}\backslash[0,\infty)$ пусть

$$R_\lambda(x,y) = \begin{cases} -\frac{f_1(x,k)f_2(y,k)}{2ika(k)}, & \text{если } x \geqslant y, \\ -\frac{f_1(y,k)f_2(x,k)}{2ika(k)}, & \text{если } x \leqslant y, \end{cases}$$

где ветвь функции $k = \sqrt{\lambda}$ на $\mathbb{C}\backslash[0,\infty)$ определяется условием, что $\operatorname{Im} k > 0$. При фиксированных x и y функция $R_\lambda(x,y)$ мероморфна на $\mathbb{C}\backslash[0,\infty)$ и имеет простые полюса в точках $\lambda_l = -\varkappa_l^2, l = 1, ..., n$.

Лемма 2.1. Оператор H самосопряжен и $R_\lambda = (H - \lambda I)^{-1}$ при $\lambda \in$ $\in \mathbb{C}\backslash\left\{[0,\infty) \cup \{\lambda_1, ..., \lambda_n\}\right\}$, где I-тождественный оператор в $L^2(\mathbb{R})$.

Теорема 2.3. Оператор $\mathscr{U}$ продолжается до оператора частичной изометрии $\mathscr{U} : \mathscr{H} \to \mathfrak{H}_0$

$$\mathscr{U}^*\mathscr{U} = I - P \quad \text{и} \quad \mathscr{U}\mathscr{U}^* = I_0,$$

и устанавливает изоморфизм $(I-P)\mathscr{H} \simeq \mathfrak{H}_0$. Здесь I и I_0 - соответственно тождественные операторы в $\mathscr{H}$ и $\mathfrak{H}_0$. Для спектра соответствующего оператора Шрёдингера H имеем $\sigma(H) = \{-\varkappa_1^2, ..., -\varkappa_n^2\} \cup \cup[0, \infty)u$

$$\mathscr{H} = \mathscr{H}_{\text{pp}} \oplus \mathscr{H}_{\text{ac}}$$

где $\mathscr{H}_{\text{pp}} = P\mathscr{H}$ и $\mathscr{H}_{\text{ac}} = (I - P)\mathscr{H}$ - соответственно инвариантные подпространства, связанные с чисто точечным и абсолютно непрерывным спектрами H. Оператор $\mathscr{U}H\mathscr{U}^*$ - это оператор умножения на λ в $\mathfrak{H}_0$, так что абсолютно непрерывный спектр $[0, \infty)$ оператора H имеет кратность два, а оператор $\mathscr{U}$ «диагонализует» ограничение H на подпространство $\mathscr{H}_{\text{ac}}$.

Следствие 2.4. Ограничение H на абсолютно непрерывное подпространство $\mathscr{H}_{\text{ac}}$ унитарно эквивалентно H_0:

$$H|_{\mathscr{H}_{\mathbf{ac}}} = UH_0U^{-1}.$$

О свободной квантовой частице в искривленном пространстве

На римановом многообразии (M, g): фазовое пространство классической частицы массы $m = 1$ - это кокасательное расслоение T^*M, и $H_{\text{c}}(\boldsymbol{p}, \boldsymbol{x}) = \frac{1}{2}g^{\mu\nu}(\boldsymbol{x})p_\mu p_\nu$, где $g^{\mu\nu}(\boldsymbol{x})$ - тензор, обратный к $g_{\mu\nu}(\boldsymbol{x})$, а $(\boldsymbol{p}, \boldsymbol{x}) = (p_1, ..., p_n, x^1, ..., x^n)$ - координаты на T^*M.

Гильбертово пространство квантовой системы - это $\mathscr{H} = L^2(M, d\mu)$, где $d\mu = \sqrt{g(\boldsymbol{x})}d^n\boldsymbol{x}, g(\boldsymbol{x}) = \det\left(g_{\mu\nu}(\boldsymbol{x})\right)$, - мера, ассоциированная с плотностью римановой метрики (римановой формы объема, если M ориентировано). Когда канонические координаты $(\boldsymbol{p}, \boldsymbol{x})$ определены на T^*M лишь локально, построить соответствующие операторы $\boldsymbol{P}$ и $\boldsymbol{Q}$ невозможно. Тем не менее всегда можно определить оператор Гамильтона

$$H = \frac{\hbar^2}{2}\Delta_g, \quad \text{где} \quad \Delta_g = -\frac{1}{\sqrt{g(\boldsymbol{x})}}\frac{\partial}{\partial x^\mu}\left(\sqrt{g(\boldsymbol{x})}g^{\mu\nu}\frac{\partial}{\partial x^\nu}\right)$$

- оператор Лапласа - Бельтрами римановой метрики g на M. Заметим, что в этом случае имеется нетривиальная задача упорядочивания некоммутирующих оператор в квантовании $H_{\text{c}}(\boldsymbol{p}, \boldsymbol{x})$, возникающая, если в координатной окрестности на M заменить канонические координаты $\boldsymbol{p}$ и $\boldsymbol{x}$ операторами $\boldsymbol{P}$ и $\boldsymbol{Q}$.

Формула $\Delta_g = -g^{\mu\nu}(\boldsymbol{x})\frac{\partial^2}{\partial x^\mu \partial x^\nu} + g^{\mu\sigma}(\boldsymbol{x})\Gamma^\nu_{\mu\sigma}(\boldsymbol{x})\frac{\partial}{\partial x^\nu}$ показывает, что самосопряженный оператор $H = \frac{\hbar^2}{2}\Delta_g$ склеивается из локальных выражений

$$H_{\text{c}}(\boldsymbol{P}, \boldsymbol{Q}) = \frac{1}{2}\left(g^{\mu\nu}(\boldsymbol{Q})P_\mu P_\nu + i\hbar g^{\mu\sigma}(\boldsymbol{Q})\Gamma^\nu_{\mu\sigma}(\boldsymbol{Q})P_\nu\right)$$

(?????????????????????? место подумать про это. мб это и так, но про это лучше еще подумать.)

Связи формализмов квантовой механики (!?!)

(очень хотелось бы иметь под рукой как раз переходы между формулизмами! тут же формализмы КТП, между ними и в квантмех тоже переходы. додумаю - напишу)

Changing from high scale to low scale models

(там такие какие-то переходы были, потом про это буду думать)

Планетарная модель атома, атом Бора-Зоммерфельда

Основные идеи планетарной модели

We can view electron as a current on contour around a nuclei and the orbit is round:

$$\mu = \frac{i}{c}S, \qquad \text{(magn mom)}$$

$$\mu = \frac{e}{c}\frac{S}{T} = \frac{e}{cT}\pi r^2 = \frac{e}{2mc}m\omega r^2 = \frac{e}{2mc}p,$$

$$\frac{\mu}{p} = \frac{e}{2mc}.$$

$$p = m\omega r^2 = n\frac{h}{2\pi}, \qquad n \in \mathbb{Z}.$$

$$\varepsilon_n = -\frac{2\pi^2 m e^4}{n^2 h^2 (1 + m/M)},$$

$$p_\varphi \to p_l = \sqrt{l(l+1)}\frac{h}{2\pi}; \quad \mu_l = \sqrt{l(l+1)}\mu_{\text{B}}$$

(?????)

Экспериментальные факты, вне рамок планетарной моделью

Тонкая структура спектральных линий вне рамок планетарной модели. При достаточно точном анализе линейчатых спектров выясняется, что почти все линии имеют тонкую структуру - состоят из ряда близких линий. При этом у щелочных металлов (Li, Na, K и т. д.) все линии двойные (дублеты), у щёлочноземельных (Be, Mg, Ca, Zn и т.д.) - простые и тройные (синглеты и триплеты), у элементов третьей группы (B, Al, Ga и т. д.) - дублеты и квартеты, у элементов четвёртой (C, Si и т. д.) синглеты, триплеты и квинтеты и т.д.

Эффект Зеемана вне рамок планетарной модели. Эффектом Зеемана называется расщепление линий при помещении излучающего вещества в магнитное поле. Оно возникает из-за изменения энергетического состояния атома вследствие взаимодействия его магнитного момента с внешним полем.

Действительно, энергия атома, помещённого в магнитное поле, равна

$$W = W_0 - \mu_H H,$$

W_0 - энергия атома при отсутствии поля. Как было указано выше (см. (1.9)), $\mu_H = -m_l\mu_{\text{B}}$; следовательно,

$$W = W_0 + \mu_{\text{B}} m_l H.$$

Таким образом, в присутствии магнитного поля состояния с различными m_l имеют различную энергию, а единый уровень энергии, отвечающий данному значению l и различным m_l, расщепляется на несколько подуровней.

Иначе говоря, вместо первоначальной линии с частотой ν_0 получаются три: одна с прежней частотой и две сдвинутые по частоте на равные расстояния по обе стороны от неё:

$$\Delta\nu = \pm\frac{\mu_{\text{B}} H}{h} = \pm\frac{eH}{4\pi mc}$$

Опыт Штерна и Герлаха вне рамок планетарной модели. (???? тут у Боровика мб ложь написана, потому что в первой группе нет некоторых металлов, которые он пишет, и вообще не нашел я за пару минут инфо про эти проверки для разных металлов, потом еще посмотрю. Пока не считаю, что этот опыт опровергает план. модель атома.) Для атомов первой группы (Li, Na, K, Cu, Ag, Au) в рамках планетарной модели полный момент равен нулю (??? почему???), но их пучок разбился на два симметрично смещённых пучка, причём из величины смещения было определено

$$\mu_H = \pm\mu_\text{B}.$$

Спин. Собственный магнитный момент электрона

(???????)

$$p_s = \sqrt{s(s+1)}\frac{h}{2\pi} = \sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right)}\frac{h}{2\pi},$$

$$\mu_{sH} = 2m_s\mu_\text{B}.$$

$$\frac{\mu_s}{p_s} = \frac{2\sqrt{s(s+1)}\mu_\text{B}}{\sqrt{s(s+1)}h/(2\pi)} = \frac{e}{mc} \equiv 2\frac{\mu}{p}$$

(????)

(!! задачи общефиза еще нарешаю ей!)

Магнитный момент атома. Фактор Ланде

$$\boldsymbol{\mu}_j = \mu_L \cos\left(\widehat{\mathbf{P}_L\mathbf{P}_J}\right) + \mu_S \cos\left(\widehat{\mathbf{P}_S\mathbf{P}_J}\right);$$

$$\mu_L = \sqrt{L(L+1)}\mu_\text{B}$$

$$\mu_S = 2\sqrt{S(S+1)}\mu_\text{B}$$

$$\begin{cases} \cos\left(\widehat{\mathbf{P}_L\mathbf{P}_J}\right) = \frac{L(L+1)+J(J+1)-S(S+1)}{2\sqrt{L(L+1)}\sqrt{J(J+1)}}, \\ \cos\left(\widehat{\mathbf{P}_S\mathbf{P}_J}\right) = \frac{S(S+1)+J(J+1)-L(L+1)}{2\sqrt{S(S+1)}\sqrt{J(J+1)}}. \end{cases}$$

$$g = 1 + \frac{J(J+1)+S(S+1)-L(L+1)}{2J(J+1)}$$

21.3.8 Quantum Fields and the Poincaré Group (!?!??!)

(напишу суть этого, очень важные темы, подробнее в теорполе или отдельной записи)

21.3.9 What can be and what cannot be in QM? (???)

(можно ли нарушать ЗСЭ? все такое. большие вопросы.)

21.3.10 Special Quantization Methods

О операторах рождения и уничтожения (??)

(??? пройду потом, пока мало с ними работал, но это важно. задачи порешаю, запишу в раздел про операторы их, про них есть задачи!)

О квантовании через правило Бора-Зоммерфельда

(!!! потренируюсь на задачах еще!!!)

$$\oint pdq = 2\pi\hbar\left(n + \frac{1}{2}\right)$$

где $n \geq 0, \in Z$, и интегрирование ведется по замкну той орбите в фазовом пространстве $\mathbb{R}^2$. (??? для каких систем это так???)

Для вполне интегрируемым гамильтоновым системам (??)с несколькими степенями свободы (см. раздел 1.2.6 главы 1). А именно: пусть $F_1 = H_c, ..., F_N - N$ независимых интегралов движения в инволюции. Правила квантования БВЗ - это

$$\oint_\gamma \boldsymbol{p}d\boldsymbol{q} = 2\pi\hbar\left(n_\gamma + \frac{1}{4}\,\mathrm{ind}\,\gamma\right),$$

где интегрирование ведется по всем 1-циклам γ в лагранжевом подмногообразии $\Lambda = \left\{(\boldsymbol{p},\boldsymbol{q}) \in \mathbb{R}^{2\boldsymbol{N}} : H_c(\boldsymbol{p},\boldsymbol{q}) = E, F_2(\boldsymbol{p},\boldsymbol{q}) = E_2, ..., F_N(\boldsymbol{p},\boldsymbol{q}) = E_N\right\}$, $\mathrm{ind}\,\gamma \in \mathbb{Z}$ - индекс Маслова цикла γ в Λ. В одно-

Правила БЗ дают только асимптотику уровней энергии при $\hbar \to 0$, однако для интегрируемых систем с дополнительной симметрией, таких как гармонический осциллятор или задача Кеплера, они определяют уровни энергии точно.

О квантовании через функцию Грина

(сомнительный метод)
(когда нужно? все такое?)
Пусть у нас есть частица, которая описывается уравнением Гамильтона:
...
Запишем для такой частицы уравнение Шредингера
...
Далее для него напишем уравнение на функцию Грина:

$$(i\hbar\partial_t - \hat{H})G(t_0, x_0, t, x) = \delta(t - t_0)\delta(x - x_0)$$

Решим это уравнение, перейдя к фурье-образу: $G(..) =$
(короче, спишу у Володи позже)

Примеры

О квантовании Вейля

(тут жестко, пока не разобрался, даже не знаю, как написать это в пару строк. начну пока в теории писать это.)

Пусть $\mathcal{A}_0 = \mathscr{S}(\mathbb{R}^{2n}, \mathbb{R}) \subset \mathcal{A}$ - подалгебра быстро убывающих классических наблюдаемых на $\mathbb{R}^{2n}$, а $\mathscr{A}_0 = \mathscr{A} \cap \mathscr{L}(\mathscr{H})$ - пространство ограниченных квантовых наблюдаемых.

Предложение 3.2. Отображение $\mathcal{A}_0 \ni f \mapsto \Phi(f) \in \mathscr{A}_0$ является квантованием, т.е. оно удовлетворяет условию

$$\lim_{\hbar\to 0} \frac{1}{2}\Phi^{-1}\left(\Phi\left(f_1\right)\Phi\left(f_2\right)+\Phi\left(f_2\right)\Phi\left(f_1\right)\right)=f_1 f_2$$

и принципу соответствия

$$\lim_{\hbar\to 0} \Phi^{-1}\left(\left\{\Phi\left(f_1\right),\Phi\left(f_2\right)\right\}_\hbar\right)=\left\{f_1,f_2\right\}, \quad f_1,f_2\in\mathcal{A}_0,$$

где

$$\left\{\Phi\left(f_1\right),\Phi\left(f_2\right)\right\}_\hbar := \frac{i}{\hbar}\left[\Phi\left(f_1\right),\Phi\left(f_2\right)\right] \qquad u \qquad \left\{f_1,f_2\right\} := \frac{\partial f_1}{\partial \boldsymbol{p}}\frac{\partial f_2}{\partial \boldsymbol{q}}-\frac{\partial f_1}{\partial \boldsymbol{q}}\frac{\partial f_2}{\partial \boldsymbol{p}}$$

- квантовая скобка и скобка Пуассона соответственно.

Квантование, связанное с отображением $\Phi = W\circ\mathscr{F}-1$, называется квантованием Вейля.

Соответствие $f\mapsto\Phi(f)$ можно легко продолжить на векторное пространство $\widehat{L^1\left(\mathbb{R}^{2n}\right)}$ - образ $L^1\left(\mathbb{R}^{2n}\right)$ при преобразовании Фурье, лежащий в пространстве $C\left(\mathbb{R}^{2n}\right)$. В более общем виде для $f\in\in\mathscr{S}\left(\mathbb{R}^{2n}\right)'$ - пространству обобщенных функций медленного роста на $\mathbb{R}^{2n}$ - соответствующее ядро

$$K\left(\boldsymbol{q},\boldsymbol{q}'\right)=\frac{1}{(2\pi\hbar)^n}\int\limits_{\mathbb{R}^n} f\left(\boldsymbol{p},\frac{\boldsymbol{q}+\boldsymbol{q}'}{2}\right)e^{\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{q}-\boldsymbol{q}')}d^n\boldsymbol{p},$$

рассматриваемое как обобщенная функция медленного роста на $\mathbb{R}^n\times\mathbb{R}^n$, является ядром Шварца линейного оператора

$$\Phi(f):\mathscr{S}\left(\mathbb{R}^n\right)\to\mathscr{S}\left(\mathbb{R}^n\right)'.$$

В частности, постоянная функция $f=1$ соответствует тождественному оператору I с ядром $K\left(\boldsymbol{q},\boldsymbol{q}'\right)=\delta\left(\boldsymbol{q}-\boldsymbol{q}'\right)$. В терминах ядра $K\left(\boldsymbol{q},\boldsymbol{q}'\right)$ формула обращения Вейля принимает вид

$$f(\boldsymbol{p},\boldsymbol{q})=\int\limits_{\mathbb{R}^n} K\left(\boldsymbol{q}-\frac{1}{2}\boldsymbol{v},\boldsymbol{q}+\frac{1}{2}\boldsymbol{v}\right)e^{\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{v}}d^n\boldsymbol{v}.$$

Обобщенная функция $f(\boldsymbol{p},\boldsymbol{q})$, определенная равенством (3.12), называется вейлевским символом оператора в $L^2\left(\mathbb{R}^n,d^n\boldsymbol{q}\right)$ с ядром Шварца $K\left(\boldsymbol{q},\boldsymbol{q}'\right)$.

Предложение 3.1. Подпространство $\operatorname{Im}\Phi\subset\mathscr{L}(\mathscr{H})$ состоит из операторов $B\in\mathscr{S}_1$, таких, что соответствующие функиии $g(\boldsymbol{u},\boldsymbol{v})=\hbar^n\operatorname{Tr}\left(BS(\boldsymbol{u},\boldsymbol{v})^{-1}\right)$ принадлежат классу Шварца $\mathscr{S}\left(\mathbb{R}^{2n}\right)$; в этом случае $W(g)=B$. Обратное отображение $\Phi^{-1}=\mathscr{F}\circ W^{-1}$ дается формулой обращения Вейля

$$\check{f}(\boldsymbol{u},\boldsymbol{v})=\hbar^n\operatorname{Tr}\left(\Phi(f)S(\boldsymbol{u},\boldsymbol{v})^{-1}\right), \quad f\in\mathscr{S}\left(\mathbb{R}^{2n}\right).$$

(?????)

Следствие 3.3.

$$\operatorname{Tr}\Phi(f)=\frac{1}{(2\pi\hbar)^n}\int\limits_{\mathbb{R}^{2n}} f(\boldsymbol{p},\boldsymbol{q})d^n\boldsymbol{p}d^n\boldsymbol{q}$$

О других квантованиях

(тут лишь укажу их, только по потребности буду разбираться нормально)

(???? где каждое нужно??? допишу потом в конце раздела. пока не знаю.)

О $qp-$квантовании (????)

Вдобавок к квантованию Вейля Φ рассмотрим также отображения $\Phi_1 : \mathscr{S}(\mathbb{R}^{2n}) \to \mathscr{L}(\mathscr{H})$ и $\Phi_2 : \mathscr{S}(\mathbb{R}^{2n}) \to \mathscr{L}(\mathscr{H})$, определяемые формулами

$$\Phi_1(f) = \frac{1}{(2\pi)^n} \int\limits_{\mathbb{R}^{2n}} \check{f}(\boldsymbol{u},\boldsymbol{v}) e^{\frac{i\hbar}{2}\boldsymbol{u}v} S(\boldsymbol{u},\boldsymbol{v}) d^n\boldsymbol{u} d^n\boldsymbol{v}$$

и

$$\Phi_2(f) = \frac{1}{(2\pi)^n} \int\limits_{\mathbb{R}^{2n}} \check{f}(\boldsymbol{u},\boldsymbol{v}) e^{-\frac{i\hbar}{2}\boldsymbol{u}\boldsymbol{v}} S(\boldsymbol{u},\boldsymbol{v}) d^n\boldsymbol{u} d^n\boldsymbol{v},$$

где $\check{f} = \mathscr{F}^{-1}(f)$ - обратное преобразование Фурье. Хотя Φ_1 и Φ_2 уже не отображают $\mathcal{A}_0$ в вещественное векторное пространство $\mathscr{A}_0$ ограниченных квантовых наблюдаемых, они удовлетворяют всем свойствам из предложения 3.2. Из (3.5) следует, что для $f \in \mathscr{S}(\mathbb{R}^{2n})$ операторы $\Phi_1(f)$ и $\Phi_2(f)$ являются интегральными операторами с интегральными ядрами:

$$K_1(\boldsymbol{q},\boldsymbol{q}') = \frac{1}{(2\pi\hbar)^n} \int\limits_{\mathbb{R}^n} f(\boldsymbol{p},\boldsymbol{q}')\, e^{\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{q}-\boldsymbol{q}')} d^n\boldsymbol{p}$$

И

$$K_2(\boldsymbol{q},\boldsymbol{q}') = \frac{1}{(2\pi\hbar)^n} \int\limits_{\mathbb{R}^n} f(\boldsymbol{p},\boldsymbol{q}) e^{\frac{i}{\hbar}\boldsymbol{p}(\boldsymbol{q}-\boldsymbol{q}')} d^n\boldsymbol{p}$$

соответственно. Как и в случае квантования Вейля, эти формулы продолжают отображения $f \mapsto \Phi_1(f)$ и $f \mapsto \Phi_2(f)$ пространства $\mathscr{S}(\mathbb{R}^{2n})'$ обобщенных функций умеренного роста на $\mathbb{R}^{2n}$. В частности, если $f(\boldsymbol{p},\boldsymbol{q})$ - полиномиальная функция (3.13), то

$$\Phi_1(f) = \sum_{|\alpha|,|\beta|\leqslant N} c_{\alpha\beta} \boldsymbol{P}^\alpha \boldsymbol{Q}^\beta$$

и

$$\Phi_2(f) = \sum_{|\alpha|,|\beta|\leqslant N} c_{\alpha\beta} \boldsymbol{Q}^\beta \boldsymbol{P}^\alpha.$$

Поэтому отображение $f \mapsto \Phi_1(f)$ называется $\boldsymbol{pq}$-квантованием, а отображение $f \mapsto \Phi_2(f) - \boldsymbol{qp}$-квантованием. Соответствующие формулы обращения -

$$f(\boldsymbol{p},\boldsymbol{q}) = \int\limits_{\mathbb{R}^n} K_1(\boldsymbol{q}-\boldsymbol{v},\boldsymbol{q}) e^{\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{v}} d^n\boldsymbol{v}$$

и

$$f(\boldsymbol{p},\boldsymbol{q}) = \int\limits_{\mathbb{R}^n} K_2(\boldsymbol{q},\boldsymbol{q}+\boldsymbol{v}) e^{\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{v}} d^n\boldsymbol{v}.$$

Обобщенная функция $f(\boldsymbol{p},\boldsymbol{q})$, определенная в (3.18), называется $\boldsymbol{pq}$ символом оператора с ядром Шварца $K_1(\boldsymbol{q},\boldsymbol{q}')$, а обобщенная функция $f(\boldsymbol{p},\boldsymbol{q})$, определенная в (3.19), $-\boldsymbol{qp}$-символом оператора с ядром Шварца $K_2(\boldsymbol{q},\boldsymbol{q}')$. Эти символы повсеместно используются в теории псевдодифференциальных операторов. Из (3.18) и (3.19) следует, что если $f(\boldsymbol{p},\boldsymbol{q}) - \boldsymbol{pq}$-символ оператора $\Phi_1(f)$, то $\overline{f(\boldsymbol{p},\boldsymbol{q})} - \boldsymbol{qp}$-символ сопряженного оператора $\Phi_1(f)^*$.

О деформационном квантовании (???)

Пусть $\mathcal{A}$ - $\mathbb{C}$-алгебра (или ассоциативная алгебра с единицей над полем k характеристики ноль) с билинейным отображением умножения $m_0 : \mathcal{A} \otimes_{\mathbb{C}} \mathcal{A} \to \mathcal{A}$, которое мы будем кратко записывать как $a \cdot b = m_0(a, b)$. Обозначим как $\mathbb{C}[[t]]$ кольцо формальных степенных рядов от t с коэффициентами из $\mathbb{C}$,

$$\mathbb{C}[[t]] = \left\{ \sum_{n=0}^{\infty} a_n t^n : a_n \in \mathbb{C} \right\},$$

и пусть $\mathcal{A}_t = \mathcal{A}[[t]]$ - это $\mathbb{C}[[t]]$-алгебра формальных степенных рядов от t с коэффициентами из $\mathcal{A}$. мы будем также обозначать m_0. Алгебра $\mathcal{A}_t\mathbb{Z}$-градуирована,

$$\mathcal{A}_t = \bigoplus_{n=0}^{\infty} A_n$$

где $A_n = t^n\mathcal{A}$, так что $A_m \cdot A_m \subset A_{m+n}$.

Определение. Формальная деформачия $\mathbb{C}$-алгебры $\mathcal{A}$ с умножением m_0 это ассоциативная алгебра $\mathcal{A}_t$ над кольцом $\mathbb{C}[[t]]$ с $\mathbb{C}[[t]]$-билинейным отображением умножения $m_t : \mathcal{A}_t \otimes_{\mathbb{C}[[t]]} \mathcal{A}_t \to \mathcal{A}_t$, таким, что

$$m_t(a, b) = a \cdot b + \sum_{n=1}^{\infty} t^n m_n(a, b)$$

для всех $a, b \in \mathcal{A}$, где $m_n : \mathcal{A} \otimes_{\mathbb{C}} \mathcal{A} \to \mathcal{A}$ - билинейные отображения.

Определение. Две формальные деформации m_t и $\tilde{m}_t\mathbb{C}$-алгебры $\mathcal{A}$ эквивалентны, если существует $\mathbb{C}[[t]]$-линейное отображение $F_t : \mathcal{A}_t \to \mathcal{A}_t$, такое, что (i) для любого $a \in \mathcal{A}$

$$F_t(a) = a + \sum_{n=1}^{\infty} t^n f_n(a)$$

где $f_n : \mathcal{A} \to \mathcal{A}$ - линейные отображения; (ii) для любых $a, b \in \mathcal{A}$

$$F_t\left(\tilde{m}_t(a, b)\right) = m_t\left(F_t(a), F_t(b)\right).$$

Определение. Коцепной комплекс Хохшильда $\mathrm{C}^\bullet(\mathcal{A}, M)\mathbb{C}$-алгебры $\mathcal{A}$ с коэффициентами в $\mathcal{A}$-бимодуле M определяется коцепями

$$\mathrm{C}^n(\mathcal{A}, M) = \mathrm{Hom}_{\mathbb{C}}\left(\mathcal{A}^{\otimes n}, M\right)$$

т. е. n-линейными отображениями $f\left(a_1, ..., a_n\right)$, определенными на $\mathcal{A}$ со значениями в M, и дифференциалом $d_n : \mathrm{C}^n(\mathcal{A}, M) \to \mathrm{C}^{n+1}(\mathcal{A}, M)$,

$$\begin{aligned}
&\left(d_n f\right)\left(a_1, a_2, ..., a_{n+1}\right) = a_1 \cdot f\left(a_2, ..., a_{n+1}\right) + \\
&+ \sum_{j=1}^{n} (-1)^j f\left(a_1, ..., a_{j-1}, a_j \cdot a_{j+1}, a_{j+2}..., a_{n+1}\right) + \\
&+ (-1)^{n+1} f\left(a_1, ..., a_n\right) \cdot a_{n+1}.
\end{aligned}$$

Имеем $d^2 = 0$, т. е. $d_{n+1} \circ d_n = 0$, и когомологии $H^\bullet(\mathcal{A}, M)$ комплекса $(\mathrm{C}^\bullet(\mathcal{A}, M), d)$,

$$H^n(\mathcal{A}, M) = \ker d_n / \operatorname{Im} d_{n-1},$$

называются когомологиями Хохшильда алгебры $\mathcal{A}$ с коэффициентами в $\mathcal{A}$ бимодуле M.

Лемма 3.3. Формальная деформачия $\mathcal{A}_t$ коммутативной $\mathbb{C}$-алгебры $\mathcal{A}$ оснащает $\mathcal{A}$ структурой алгебры Пуассона со скобкой $\{,\}$.

Определение. Деформационное квантование алгебры Пуассона $(\mathcal{A}, \{\},)$ с коммутативным произведением $m_0 : \mathcal{A} \otimes_{\mathbb{C}} \mathcal{A} \to \mathcal{A}$ - это формальная деформация $\mathcal{A}_t$ алгебры $\mathcal{A}$, такая, что отображение умножения m_t удовлетворяет (3.28).

По лемме 3.3 любая формальная деформация $\mathcal{A}_t$ коммутативной алгебры $\mathcal{A}$ является деформационным квантованием алгебры Пуассона $(\mathcal{A}, \{\}$, со скобкой Пуассона, заданной формулой (3.27).

Согласно лемме 3.2, деформационное квантование алгебры Пуассона $(\mathscr{S}(\mathbb{R}^{2n}), \{\},)$, в которой скобка Пуассона ассоциирована с канонической симплектической формой $\omega = d\boldsymbol{p} \wedge d\boldsymbol{q}$, есть алгебра $\mathscr{S}(\mathbb{R}^{2n})[[t]]$, где $t = -i\hbar$, а $\hbar$ рассматривается как формальный параметр, и отображение умножения дается $\star$-произведением. Следующее утверждение - формальный алгебраический аналог представления (3.22) для $\star$-произведения. Теорема 3.4 (Универсальная деформация). Пусть $\mathcal{A}$ - коммутативная $\mathbb{C}$-алгебра с отображением умножения m_0 и пусть $\varphi_1 \boldsymbol{u} \varphi_2$ - два коммутируючих дифференцирования алгебры $\mathcal{A}$, т.е. линейных отображения $\varphi_1, \varphi_2 : \mathcal{A} \to \mathcal{A}$, удовлетворяющих правилу Лейбница и условию

$$\varphi_1 \circ \varphi_2 = \varphi_2 \circ \varphi_1.$$

Тогда выражение

$$\{a, b\} = \varphi_1(a) \cdot \varphi_2(b) - \varphi_2(a) \cdot \varphi_1(b), \quad a, b \in \mathcal{A},$$

определяет на $\mathcal{A}$ скобку Пуассона, и формулой

$$m_t = m_0 \circ e^{t\Phi}, \quad \Phi = \varphi_1 \otimes \varphi_2,$$

называемой формулой универсальной деформачии, дается деформачионное квантование алгебры Пуассона $(\mathcal{A}, \{\})$.

21.4 Methods for special applications 1

21.4.1 Rotations, C-, P-, T-Symmetry

О Т-четности и обращении времени

Main methods

(нужно отдельно про это почитать!!!)

$$\Theta \mathbf{x} \Theta^\dagger = \mathbf{x}, \quad \Theta \mathbf{p} \Theta^\dagger = -\mathbf{p}$$
$$\Theta H \Theta^\dagger = H \quad \text{or} \quad [\Theta, H] = 0$$

Because if $\tau = -t$, so $|\psi_r(t)\rangle = \Theta|\psi(\tau)\rangle$, then

$$i\hbar \frac{\partial}{\partial t} |\psi_r(t)\rangle = \Theta \left[i\hbar \frac{\partial}{\partial \tau} |\psi(\tau)\rangle \right] = \Theta H |\psi(\tau)\rangle = \left(\Theta H \Theta^\dagger\right) \Theta |\psi(\tau)\rangle = \left(\Theta H \Theta^\dagger\right) |\psi_r(t)\rangle$$

The time-reversal operator unitary or antiunitary:

$$T(iH)T^{-1} = -iH$$

Because if we take the canonical commutation relations, $[x_i, p_j] = i\hbar\delta_{ij}$, and conjugate with Θ, we find $\Theta [x_i, p_j] \Theta^\dagger = -[x_i, p_j] = -i\hbar\delta_{ij} = \Theta (i\hbar\delta_{ij}) \Theta^\dagger$ The quantity $i\hbar\delta_{ij}$ is just a number, so if Θ is unitary it can be brought through to cancel $\Theta^\dagger$, and we obtain a contradiction.

Time reversibility by Zhou

$$|\psi_r(t)\rangle = \Theta|\psi(-t)\rangle$$

$$\Theta^\dagger\Theta = 1$$

$$\Theta\mathbf{x}\Theta^\dagger = \mathbf{x}, \quad \Theta\mathbf{p}\Theta^\dagger = -\mathbf{p}$$

$$\Theta[x,p]\Theta^\dagger = i\hbar\Theta\Theta^\dagger = i\hbar = [x,p]$$

Applications of time reversibility (????)

(очень много про это написано, потом продумаю)

О P-четности и инверсии пространства

Parity by Zhou

$$\pi^\dagger\pi = 1, \quad \pi^2 = 1, \quad \pi U(R)\pi^\dagger = U(R)$$

$$\pi\mathbf{x}\pi^\dagger = -\mathbf{x}, \quad \pi\mathbf{p}\pi^\dagger = -\mathbf{p}, \quad \pi\mathbf{L}\pi^\dagger = \mathbf{L}$$

$\mathbf{L} = \mathbf{r} \times \mathbf{p}$.
the parity of the state $|lm\rangle$ is $(-1)^l$.

Vector $\pi\mathbf{V}\pi^\dagger = \pm\mathbf{V}$ true/pseudo- v

Scalar $\pi K\pi^\dagger = \pm K$ true/pseudo- s

Applications of P-четности (????)

вроде задачу с диполем можно вписать

О C-симметрии (???)

О CPT симметрии (???)

О других дискретных симметриях

О d-функции Вигнера

(все про нее, мб Вайнбегра почитаю даже, пок ане до нее)

О другом про симметрии пространства (??)

(там просто много всего, так что могу указать это потом)

О важности и применениях дискретных симметрий (??)

(укажу, зачем вообще ими заниматься?? обзор вообще применений всех их, самые важные применения укажу)

21.4.2 Symmetries, group theory methods

(см. пока книгу Ландау, очень много что можно делать, не владея этим.)

§91. Symmetry transformations 356

§92. Transformation groups 359

§93. Point groups 362

§94. Representations of groups 370

§95. Irreducible representations of point groups 378

§96. Irreducible representations and the classification of terms 382

§97. Selection rules for matrix elements 385

§98. Continuous groups 389

§99. Two-valued representations of finite point groups

21.4.3 Sepcial mathematical constructions by Takhtajan

(??? пока не до них было)

О соотношении и преобразовании Вейля

$$W(f) = \frac{1}{(2\pi)^n} \int\limits_{\mathbb{R}^{2n}} f(\boldsymbol{u}, \boldsymbol{v}) e^{-i(\boldsymbol{u}\boldsymbol{P}+\boldsymbol{v}\boldsymbol{Q})} d^n\boldsymbol{u} d^n\boldsymbol{v}$$

Пусть R - неприводимое унитарное представление группы Гейзенберга $\mathbf{H}_n$ в гильбертовом пространстве $\mathscr{H}$. Из леммы Шура следует, что $R(e^{\alpha c}) = e^{i\hbar\alpha} I$ для некоторого $\hbar \in \mathbb{R}$, где I - тождественный оператор в $\mathscr{H}$. Если $\hbar = 0, n$-параметрические абелевы группы унитарных операторов $U(\boldsymbol{u}) = R\left(e^{\boldsymbol{u}X}\right)$ и $V(\boldsymbol{v}) = R\left(e^{\boldsymbol{v}Y}\right)$ коммутируют, так что, еще раз воспользовавшись леммой Шура, заключаем, что существуют $\boldsymbol{p}, \boldsymbol{q} \in \mathbb{R}^n$, такие, что $U(\boldsymbol{u}) = e^{-i\boldsymbol{u}\boldsymbol{p}} I$ и $V(\boldsymbol{v}) = e^{-i\boldsymbol{v}\boldsymbol{q}} I$. Потому в этом случае неприводимое представление R одномерно и параметризуется вектором $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{R}^{2n}$. Когда $\hbar \neq 0$, унитарные операторы $U(\boldsymbol{u})$ и $V(\boldsymbol{v})$ удовлетворяют соотношениям Вейля

$$U(\boldsymbol{u})V(\boldsymbol{v}) = e^{i\hbar uv} V(\boldsymbol{v})U(\boldsymbol{u}),$$

допускающим представление Шрёдингера, введенное в разделе 2.2.2. Оказывается, что любое неприводимое представление группы Гейзенберга $\mathbf{H}_n$ унитарно эквивалентно либо одномерному представлению с параметрами $(\boldsymbol{p}, \boldsymbol{q}) \in \mathbb{R}^{2n}$, либо представлению Шрёдингера для какого-то $\hbar \neq 0$. Физически осмысленный случай соответствует значению $\hbar > 0$, и представление с $-\hbar$ дается операторами $U^{-1}(\boldsymbol{u}) = U(-\boldsymbol{u})$ и $V(\boldsymbol{v})$.

Теорема Стоуна-фон Неймана: Любое неприводимое унитарное представление соотношений Вейля для n степеней свободы, $U(\boldsymbol{u})V(\boldsymbol{v}) = e^{i\hbar\boldsymbol{u}v} V(\boldsymbol{v})U(\boldsymbol{u})$ унитарно эквивалентно представлению Шрёдингера.

Определим линейное отображение $W : L^1(\mathbb{R}^2) \to \mathscr{L}(\mathscr{H})$, называемое преобразованием Вейля, по формуле

$$W(f) = \frac{1}{2\pi} \int\limits_{\mathbb{R}^2} f(u, v) S(u, v) du dv.$$

Здесь интеграл понимается в слабом смысле: для любого $\psi_1, \psi_2 \in \mathscr{H}$

$$(W(f)\psi_1, \psi_2) = \frac{1}{2\pi} \int\limits_{\mathbb{R}^2} f(u,v)\,(S(u,v)\psi_1, \psi_2)\,dudv$$

Преобразование Вейля обладает следующими свойствами.

WT1. Для $f \in L^1(\mathbb{R}^2)$

$$W(f)^* = W(f^*)$$

где $f^*(u,v) = \overline{f(-u,-v)}$.

WT2. Для $f \in L^1(\mathbb{R}^2)$

$$S(u_1,v_1)\,W(f)S(u_2,v_2) = W(\tilde{f}),$$

где $\tilde{f}(u,v) = e^{\frac{i\hbar}{2}\{(u_1-u_2)v-(v_1-v_2)u+u_1v_2-u_2v_1\}} f(u-u_1-u_2, v-v_1-v_2)$.

WT3. $\operatorname{Ker} W = \{0\}$.

WT4. Для $f_1, f_2 \in L^1(\mathbb{R}^2)$

$$W(f_1)\,W(f_2) = W(f_1 *_\hbar f_2),$$

где $(f_1 *_\hbar f_2)(u,v) = \frac{1}{2\pi} \int\limits_{\mathbb{R}^2} e^{\frac{i\hbar}{2}(uv'-u'v)} f_1(u-u', v-v')\,f_2(u',v')\,du'dv'$.

Таким образом, преобразование Вейля

$$W(f) = \frac{1}{(2\pi)^n} \int\limits_{\mathbb{R}^{2n}} f(\boldsymbol{u},\boldsymbol{v}) e^{-i(\boldsymbol{uP}+\boldsymbol{vQ})} d^n\boldsymbol{u}\,d^n\boldsymbol{v}$$

можно рассматривать как некоммутативное преобразование Фурье - операторнозначное обобщение «обычного» преобразования Фурье

$$\hat{f}(\boldsymbol{p},\boldsymbol{q}) = \frac{1}{(2\pi)^n} \int\limits_{\mathbb{R}^{2n}} f(\boldsymbol{u},\boldsymbol{v}) e^{-i(\boldsymbol{up}+\boldsymbol{vq})} d^n\boldsymbol{u}\,d^n\boldsymbol{v}$$

(???? подумаю про это!!!!)

Лемма 3.1. Преобразование Вейля W определяет изоморфизм $L^2(\mathbb{R}^{2n}) \simeq \mathscr{S}_2$

Бескоординатное представление Шредингера по Тахтаджаяну (?????)

(!!! в 1/3 страницы сверну это, не больше, это прикольно, но бесполезно!!!)

Пусть (V,ω) - конечномерное симплектическое векторное пространство, $\dim V = 2n$. Напомним, что (см. раздел 2.2.1) алгебра Гейзенберга $\mathfrak{g} = \mathfrak{g}(V)$ - это одномерное центральное расширение абелевой алгебры Ли V с помощью кососимметрической билинейной формы ω. Как векторное пространство алгебра Ли $\mathfrak{g}$ совпадает с алгеброй $V \oplus \mathbb{R}$, в которой скобка Ли определена равенством

$$[u+\alpha c, v+\beta c] = \omega(u,v)c, \quad u,v \in V, \alpha,\beta \in \mathbb{R}.$$

Любое лагранжево подпространство ℓ пространства V определяет абелеву подалгебру $\ell \oplus \mathbb{R}c$ в $\mathfrak{g}$. Лагранжево подпространство ℓ' дополнительно к ℓ в V, если $\ell \oplus \ell' = V$. Выбором дополнительного к ℓ лагранжева подпространства ℓ' устанавливается изоморфизм

$$\mathfrak{g}/(\ell \oplus \mathbb{R}c) \simeq \ell'$$

Группа Гейзенберга $G = G(V)$ - связная и односвязная группа Ли с алгеброй Ли g. Экспоненциальным отображением осуществляется изоморфизм G и многообразия $V \oplus \mathbb{R}c$, в котором групповой закон задан равенством

$$\exp(v_1 + \alpha_1 c)\exp(v_2 + \alpha_2 c) = \exp\left(v_1 + v_2 + \left(\alpha_1 + \alpha_2 + \frac{1}{2}\omega(v_1, v_2)\right)c\right),$$

где $v_1, v_2 \in V, \alpha_1, \alpha_2 \in \mathbb{R}$. Выбором симплектического базиса для V устанавливается изоморфизм $G(V) \simeq \mathbf{H}_n$ с матричной группой Гейзенберга, определенной в разделе 2.2.1. Форма объема $d^{2n}\boldsymbol{v} \wedge dc$, где $d^{2n}\boldsymbol{v} \in \Lambda^{2n}V^*$ - форма объема на V, а V^* - двойственное к V векторное пространство, определяет биинвариантную меру Хаара на G. Любое лагранжево подпространство ℓ определяет абелеву подгруппу $L = \exp(\ell \oplus \mathbb{R}c)$ в G, а выбором дополнительного лагранжева подмножества ℓ' устанавливается изоморфизм

$$G/L \simeq \ell'.$$

Изоморфизм $\Lambda^{2n}V^* \simeq \Lambda^n\ell^* \wedge \Lambda^n\ell'^*$ приводит к форме объема d^nv' на ℓ' и определяет меру dg на однородном пространстве G/L. Мера dg инвариантна при левом действии G и не зависит от выбора ℓ'. Для заданного $\hbar \in \mathbb{R}$ функция $\chi : L \to \mathbb{C}$,

$$\chi(\exp(v + \alpha c)) = e^{i\hbar\alpha}, \quad v \in V, \alpha \in \mathbb{R},$$

определяет одномерный унитарный характер на L,

$$\chi(l_1 l_2) = \chi(l_1)\chi(l_2), \quad l_1, l_2 \in L.$$

Определение. Бескоординатное представление Шрёдингера S_ℓ группы Гейзенберга $G(V)$, ассоциированное с лагранжевым подпространством ℓ пространства V, - это представление группы G, индуцированное одномерным представлением χ соответствующей абелевой группы Ли L,

$$S_\ell = \mathrm{Ind}_L^G \chi.$$

По определению индуцированного представления гильбертово пространство $\mathscr{H}_\ell$ представления S_ℓ состоит из измеримых функций $f : G \to \mathbb{C}$, удовлетворяющих свойству $f(gl) = \chi(l)^{-1}f(g), \quad g \in G, l \in L$, и таких, что $\|f\|^2 = \int\limits_{G/L} |f(g)|^2 dg < \infty$.

О виковском символе (???)

Представим A в виковской нормальной форме следующим образом:

$$A = \sum_{l,m} A_{lm} (a^*)^l a^m.$$

По определению виковский символ $A(\bar{z}, z)$ оператора A - это

$$A(\bar{z}, z) = \sum_{l,m} A_{lm} \bar{z}^l z^m$$

Теорема 2.2. Виковские символы ограниченных операторов в $\overline{\mathscr{D}}$ обладают следующими свойствами.

(i) Если $A(\bar{z}, z)$ - виковский символ оператора A, то для виковского символа оператора A^* имеем $A^*(\bar{z}, z) = \overline{A(\bar{z}, z)}u$

$$A^*(v, z) = \overline{A(\bar{z}, \bar{v})}$$

(ii) Для $f \in \overline{\mathscr{D}}$

$$(Af)(\bar{z}) = \frac{1}{\pi} \int\limits_{\mathbb{C}} A(\bar{z}, v) f(\bar{v}) e^{-v(\bar{v}-\bar{z})} d^2 v.$$

(iii) Вещественно-аналитическая функиия $A(\bar{z}, z)$ является виковским символом ограниченного оператора A в $\overline{\mathscr{D}}$, если и только если она есть ограничение на подпространство $v = \bar{z}$ челой функции $A(v, z)$ в переменных v и z со свойством, что для любого $f \in \mathscr{D}$ интеграл в части (ii) абсолютно сходится и определяет функиию в $\bar{D}$.

(iv) Если $A_1(\bar{z}, z)$ и $A_2(\bar{z}, z)$ - виковские символь операторов A_1 и A_2, то виковский символ оператора $A = A_1 A_2$ задается формулой

$$A(\bar{z}, z) = \frac{1}{\pi} \int\limits_{\mathbb{C}} A_1(\bar{z}, v) A_2(\bar{v}, z) e^{-(v-z)(\bar{v}-\bar{z})} d^2 v$$

Матричный символ $\tilde{A}(\bar{z}, z)$ ограниченного оператора A в гильбертовом пространстве $\mathscr{D}$ - это ограничение на подпространство $v = \bar{z}$ целой функции $A(v, z)$ в переменных v и z, определенной следующим абсолютно сходящимся рядом:

$$\tilde{A}(v, z) = \sum_{m,n=0}^{\infty} \left(A\bar{f}_m, \bar{f}_n\right) f_n(v) f_m(z).$$

Матричный и виковский символы связаны следующим образом.

Следствие 2.3. Если $\tilde{A}_1(\bar{z}, z)$ и $\tilde{A}_2(\bar{z}, z)$-матричные символы операторов A_1 и A_2, то матричный символ оператора $A = A_1 A_2$ дается формулой

$$\tilde{A}(\bar{z}, z) = \frac{1}{\pi} \int\limits_{\mathbb{C}} \tilde{A}_1(\bar{z}, v) \tilde{A}_2(\bar{v}, z) e^{-|v|^2} d^2 v$$

Лемма 2.4. Для ограниченного оператора A в гильбертовом пространстве $\bar{D}$

$$\tilde{A}(v, z) = e^{vz} A(v, z)$$

21.4.4 Symmetries in Quantum Mechanics and Their Consequences

(см. ЛЛ3, там большой раздел про это, я не много пока этим занимался. пока я очень плохо понимаю, что там происходит и как этим пользоваться?)

О правилах отбора из симметрий (!?!?)

(ЛЛ3, по идее разберусь, пару абзацев на это, пока мало думал про это.)

21.4.5 Absence of Hidden Variables, Bell's Theorem, EPR

(это большие темы, только когда основное сделано будет, будут проведены исследования и написаны статьи, буду смотреть это.)

Парадокс Эйнштейна—Подольского—Розена

(Киселев, дополнения)

О неравенстве Белла (???)

(Киселев, дополнения)

21.4.6 Response, Polarization, Susceptibility

(пока об этом в конд средах или статфизе)

О параметрах электродинамики через квантовую механику

О поляризации (!?!??)

$$\mathbf{P}(t) = \langle \chi(t) | \hat{\sigma} | \chi(t) \rangle,$$

Просто среднее значение спина (??)

О восприимчивости (??)

(там в статфизе уже про это писал, формула Кубо, отклик, все такое, потом сюда тоже добавлю, или удалю этот раздел просто, посмотрим)

21.4.7 Generalized Functions in Quantum Mechanics

(all about it here, maybe I'll merge it with some subsubsectinos of mathematics for QM)

21.4.8 Other Useful Methods for the Schrödinger Equation

Строгие математикческие методы в двух словах

(тут половина страницы на методы Константинова!!! запросто впишу, если только нужно будет!)

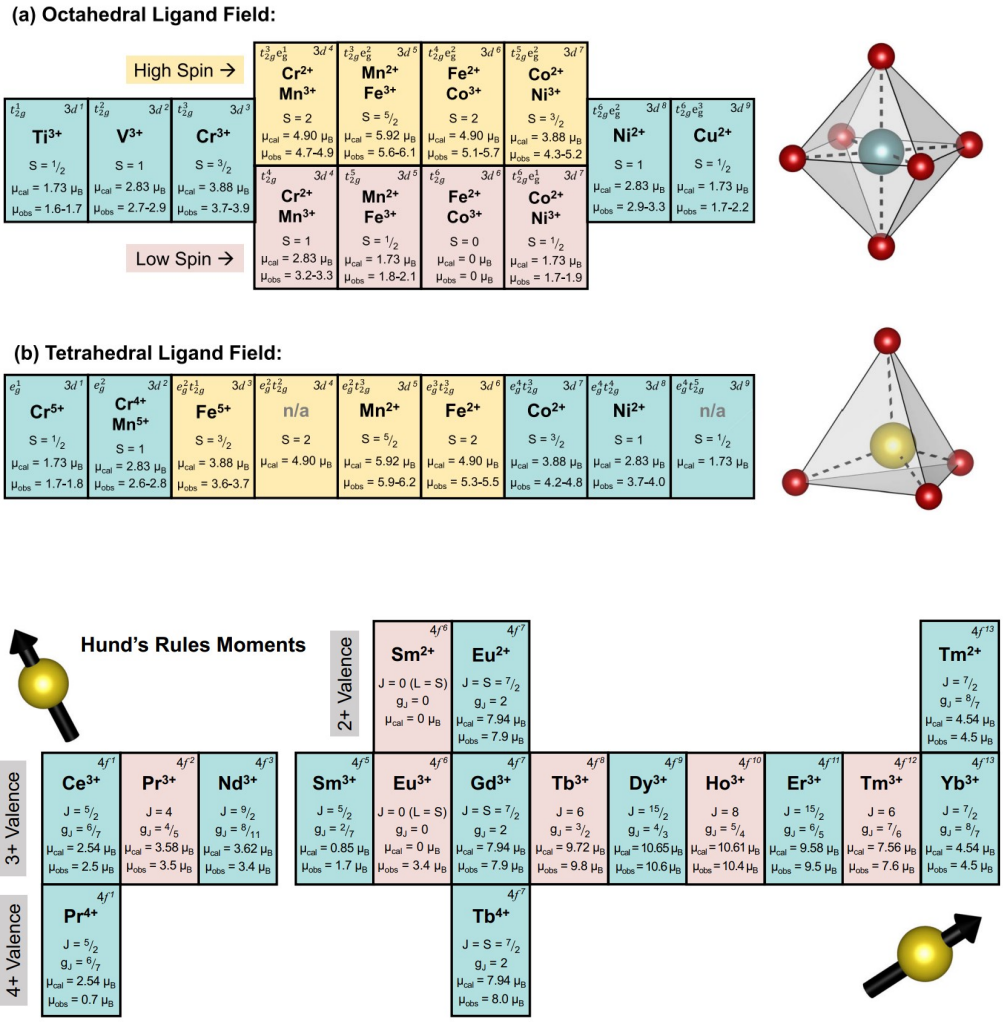
21.4.9 Other Estimates (!!!!)

(У МК много крутого еще есть, так что вот, для них раздел. мб даже пару разделов создам потом)

21.4.10 Other methods of atomic properties

Hund's rules details (????)

(в планах продумать глубже эти правила и связь с экспериментами, пока не актуально это просто)



(images from "Guide to Interpreting Magnetic Susceptibility Data with the Curie-Weiss Law" article, I'll think about them later, they are illustrating Hund's rule)

21.4.11 Perturbation theory in QM: other methods

On rigorous perturbation theory

(см. Саймонс Рид, Тахтаджаяна и многих дргуих. Это большая тема, тут просто пунктами идеи и выводы укажу, во 2й 1й части будет обзор формул. Все равно крайне маловеротяно, что они будут использоваться.)

21.5 Methods for special applications 2

21.5.1 Path integral in QM: special methods

(потом сделаю пару разделов скорее всего, пока все тут об этом.)

Основные формулы интеграла по траекториям

Суть и важность интеграла по траекториям

Об основной идее

(суть по Зи скорее всего напишу)

Основные формулы интеграла по траекториям

отличие интеграла по траекториям в квантой механики от интеграла в КТП

Примеры

(самые типичные иллюстративные добавлю)

О другом про траекториям (?)

(их очень много, но сперва пишу про них в отдельной записи)

о неверных подходах к интегралу по траекториям

про них можно говорить долго, так что лишь вкратце упомянем суть.

О Формализме Гельфанда–Яглома

(см. ПТФ, уже в этой записи написано, позже продумаю)

Об интеграле Швингера–Келдыша

(доп от Киселева, напишу потом)

21.5.2 Diagrammatic Techniques (???)

(думаю, важно указать это, все-таки много чего тут есть. но мб нет, мб в КТП это будет написано, посмотрим.)

21.5.3 Quantum information theory: Basic models

О разложениях состояний

О состояниях

- Bell States:

$$|\beta_{00}\rangle = \frac{|00\rangle+|11\rangle}{\sqrt{2}} \quad |\beta_{01}\rangle = \frac{|10\rangle+|01\rangle}{\sqrt{2}}$$
$$|\beta_{10}\rangle = \frac{|00\rangle-|11\rangle}{\sqrt{2}} \quad |\beta_{11}\rangle = \frac{|10\rangle-|01\rangle}{\sqrt{2}}$$

Параметры Стокса (????)

Разложение Шмидта (?????)

(???? укажу, что вообще происходит??? не понимаю пока)

$$\left|\psi^{AB}\right\rangle \in \mathcal{H}^A \otimes \mathcal{H}^B \quad \dim \mathcal{H}^A = d \leqslant D = \dim \mathcal{H}^B$$
$$\left|\psi^{AB}\right\rangle = \sum_{i=1}^{d}\sum_{j=1}^{D}\sum_{k=1}^{d} U_{ik}\lambda_k V_{kj}|i\rangle \otimes |j\rangle$$
$$\left|\psi^{AB}\right\rangle = \sum_{k=1}^{d} \lambda_k \left(\sum_{i=1}^{d} U_{ik}|i\rangle\right) \otimes \left(\sum_{j=1}^{D} V_{kj}|j\rangle\right)$$

Об информационной энтропии (!!!???)

О квантовых вентилях

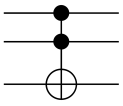
$$X_{(\text{Not})} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$H_{(\text{Hdmrd})} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \qquad S_{(\text{phase})} = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix} \qquad T = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$$

$$\begin{pmatrix} |0\rangle \\ |1\rangle \end{pmatrix}$$

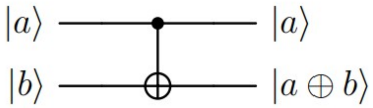
Sometimes it is more useful to work with bra-ket notation, not in matrix form.

Toffoli gate (CCNOT):

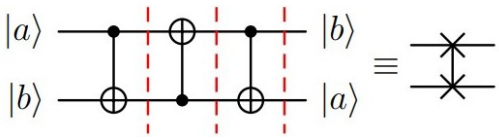


It applies the NOT if the two control qubits are 1.

cnot:



swap:



(!!! I'll add some basic methods for gates and proofs!!!!)

On some gate methods and constructions

On Quantum Fourier transform

(напишу потом на половину страницы, что да, такое есть, там соображения такие отдельные)

21.5.4 Quantum information theory: Basic theorems

(см. отдельную мою запись, а также лекции Тонга пока что, потом допишу, если будет нужно.)

21.5.5 Methods for open systems

(теория про это в 1й части, тут типичные модели, страниц мб 6-8 будет в итоге)

Спин-бозонная модель

Система (s, system) будет представлять собой двухуровневую систему (это может быть спин-1/2 в магнитном поле, это может быть частица в двухъямном потенциале - детали совершенно не важны), которую мы будем описывать на языке спина-1/2 и матриц Паули. В качестве модели окружающей среды (e, environment; также часто её называют баней - bath) мы возьмём набор гармонических осцилляторов. Гамильтониан всей системы имеет вид:

$$\hat{H} = \underbrace{-\frac{\Delta}{2}\hat{\sigma}_z}_{\hat{H}_s} + \underbrace{\sum_n \omega_n \hat{a}_n^\dagger \hat{a}_n}_{\hat{H}_e} + \underbrace{\hat{\sigma}_x \sum_n \lambda_n \hat{X}_n}_{\hat{V}}, \quad \hat{X}_n = \hat{a}_n + \hat{a}_n^\dagger$$

Система Для матриц Паули мы получаем:

$$\frac{d\hat{\sigma}_x}{dt} = i\left[\hat{H}_s, \hat{\sigma}_x\right] = \Delta\hat{\sigma}_y, \quad \frac{d\hat{\sigma}_y}{dt} = -\Delta\hat{\sigma}_x, \quad \frac{d\hat{\sigma}_z}{dt} = 0$$

и решение записывается как:

$$\begin{cases} \hat{\sigma}_x(t) = \hat{\sigma}_x \cos\Delta t + \hat{\sigma}_y \sin\Delta t \\ \hat{\sigma}_y(t) = -\hat{\sigma}_x \sin\Delta t + \hat{\sigma}_y \cos\Delta t \\ \hat{\sigma}_z(t) = \hat{\sigma}_z \end{cases}$$

Представление взаимодействия

. 102

Приближение Борна – Маркова

. 103
(тут еще формулы)
Если предположить, что этот масштаб времени много меньше масштаба времени, на котором меняется сама матрица плотности, то можно заменить $\hat{\rho}_s(t-\tau) \mapsto \hat{\rho}_s(t)$, а также в силу сходимости интеграла, заменить его верхний предел до бесконечности. В результате мы получаем следующее квантовое кинетическое уравнение (master equation):

$$\frac{d\hat{\rho}_s}{dt} = -\int_0^\infty d\tau \, \mathrm{Tr}_e\left(\left[\left[\hat{\rho}_s(t)\hat{\rho}_e, \hat{V}(t-\tau)\right], \hat{V}(t)\right]\right)$$

В таком виде это - система линейных дифференциальных уравнений с постоянными коэффициентами на компоненты матрицы плотности $\hat{\rho}_s$. Если окружающая среда не обладает памятью, то самый общий вид квантового кинетического уравнения имеет вид уравнения Линблада [4]:

$$\frac{d\hat{\rho}_s(t)}{dt} = i\left[\hat{\rho}_s(t), \hat{H}_s\right] + \mathcal{L}\hat{\rho}_s(t)$$

9.1.3

Корреляционные функции среды

105
9.1.4

Уравнения Блоха

. 105

О спектральной плотности

107

О применениях

(полстраницы словами пишу, что на самом деле это нужные темы и многое тут можно исследовать и многие этим занимаются. как конкретно?)
9.2

Подавление туннелирования в двухуровневой системе

108

Пертурбативное рассмотрение

.. 108

Адиабатическое рассмотрение

.. 108

21.5.6 Summation of many moments

(нужно будет - впишу суть)

О сложении трех моментов (???)

(тут пара крутых формул будет, важная часть теории квантмеха.)

106. 3.j-символы

107. Матричные элементы тензоров

108. 6j-символы

109. Матричные элементы при сложении моментов

110. Матричные элементы для аксиально-симметричных систем

21.5.7 Quantum chaos

non-equilibrium statistical mechanics

quantum chaos

entanglement and quantum chaos

disordered systems

21.5.8 On quantum noise (!!!!)

Essence of q noise (????)

(пока этим не занимаюсь, просто наверняка очень много приложений именно в этой теме, так что оставил заготовку. думаю, важно понимать ее для применения квантовой механики.)

21.5.9 On quantum metrology and its applications

Quantum metrology is the study of making high-resolution and highly sensitive measurements of physical parameters using quantum theory to describe the physical systems, particularly exploiting quantum entanglement and quantum squeezing.

Essence of q metrology (????)

(пока этим не занимаюсь, просто наверняка очень много приложений именно в этой теме, так что оставил заготовку. думаю, важно понимать ее для применения квантовой механики.)

22 Other Models

22.1 Famous condensed matter models

22.1.1 Electric, thermal properties of matter

О квантовании решеток и теплоемкости

Об электрических свойствах металлов

22.1.2 Famous Topological Models

Симметрии в квантовой механике для топологических систем

Симметрия по отношению к обращению времени

. 112
10.1.2

Киральная симметрия

. 113

Цепочка Su – Schrieffer – Heeger

(см. пока запись по конд средам)

Основная идея

Свойства «объёма»

10.2.2

Топологические фазы объемной задачи в термодинамическом пределе

115
10.2.3

Краевые моды

117
10.2.4

Граница между двумя топологическими фазами (состояния Jackiw – Rebbi)

.

22.1.3 Typical Magnetism in a Nutshell

(чисто квантовое явление, вот и пишу его)

Основные типы и свойства

(по идее это то же, что и в статфизе)

О диамагнитных атомах

(задачи ГК есть про это, вот тут и теория про них будет. Отдельно нужно додумывать это!!!)

22.1.4 Fundamentals of Theories of Superfluidity

(см. пока конд. среды про это, большие темы)

22.1.5 Fundamentals of Theories of Superconductivity

(см. пока конд. среды про это, большие темы)

22.1.6 Bound States in Condensates, Transport, Localization

(см. пока конд. среды про это, большие темы)

22.2 Typical models of atomic, molecule, nuclear physics

22.2.1 Review of Properties of Molecules and Methods for Them

Металлическая связь

(буду касаться химии - доучу, всё это как-то из квантмеха следует)

Ковалентная связь

Ионная связь

Ван-дер-ваальсова связь

22.2.2 Diatomic Molecules (???)

(см. ЛЛ3, нужно будет - впишу. пока там скорее энциклопедичекие сведения, чем часто используемая теория.)

Основные формулы и свойства

ЛЛ-78. Электронные термы двухатомной молекулы по Ландау

ЛЛ-79. Пересечение электронных термов по Ландау

ЛЛ-80. Связь молекулярных термов с атомными по Ландау

ЛЛ-81. Валентность по Ландау

ЛЛ-82. Колебательная и вращательная структуры синглетных термов двухатомной молекулы по Ландау

ЛЛ-83. Мультиплетные термы. Случай a по Ландау

ЛЛ-84. Мультиплетные термы. Случай b по Ландау

ЛЛ-85. Мультиплетные термы. Случаи c и d по Ландау

ЛЛ-86. Симметрия молекулярных термов по Ландау

ЛЛ-87. Матричные элементы для двухатомной молекулы по Ландау

ЛЛ-88. Λ-удвоение по Ландау

ЛЛ-89. Взаимодействие атомов на далеких расстояниях по Ландау

22.2.3 Polyatomic Molecules: Basics

(см. пока Ландау)

ЛЛ-100. Классификация молекулярных колебаний

ЛЛ-101. Колебательные уровни энергии

ЛЛ-102. Устойчивость симметричных конфигураций молекулы

ЛЛ-103. Квантование вращения волчка

ЛЛ-104. Взаимодействие колебаний и вращения молекулы

ЛЛ-105. Классификация молекулярных термов

22.2.4 Specific models of scattering of atoms and electrons

(чисто атомная физика разная)

Regge poles (!?)

(основная идея)

(осн. формулы, см. пока ЛЛ3.141)

(1 раз посижу над этим - и впишу! интересно, просто пока не нужно было, а так бы выучил!)

138. Резонансное рассеяние заряженных частиц

(см. ЛЛ3.138, на самом деле это специфика, отдельно сидеть нужно над ней)

$$\chi'' + \left(k^2 - \frac{2}{r}\right)\chi = 0$$

$$F_0{}^{ikr} krF\left(\frac{i}{k} + 1, 2, -2ikr\right), \quad A^2 = \frac{2\pi/k}{e^{2\pi/k} - 1}$$

$$F_0 \approx \sin\left[kr - \frac{1}{k}\ln(2kr) + \delta_0^{\text{кул}}\right], \quad \delta_0^{\text{кУл}} = \arg\Gamma\left(1 + \frac{i}{k}\right)$$

$r(kr \ll 1, r \ll 1)$

$$F_0 = Akr(1 + r + ...)$$

139. Упругие столкновения быстрых электронов с атомами

(см. ЛЛ3.139, на самом деле это специфика, отдельно сидеть нужно над ней)

140. Рассеяние при спин-орбитальном взаимодействии

(см. ЛЛ3.140, на самом деле это специфика, отдельно сидеть нужно над ней)

Разные конкретные известные решенные задачи

Сечение рассеяния протона на атоме водорода (151).

(порешаю по МК, впишу на 1/4 страницы суть)

22.2.5 Inelastic Collisions

(пока см. отдельную запись и книгу Ландау, не такие типичные задачи.)

Упругое рассеяние при наличии неупругих процессов

Неупругое рассеяние медленных частиц

Матрица рассеяния при наличии реакций

Формулы Брейта и Вигнера

Взаимодействие в конечном состоянии при реакциях

Поведение сечений вблизи порога реакции

Неупругие столкновения быстрых электронов с атомами

Эффективное торможение

Неупругие столкновения

22.2.6 The Essence of Typical Models of Elementary Particles

(должны задачи решаться с помощью этой главы!!!!)

Основные свойства

Все лептоны - фермионы. Нейтрино имеют только отрицательную спиральность (левоспиральные частицы), а антинейтрино - только положительную (правоспиральные).

Поколение	Частица	Символ		Масса, МэВ	Время жизни τ	Лептонный заряд			Преобладающая схема распада
		Частица	Античастица			L_e	L_μ	L_τ	
I	электрон	e^-	e^+	0,511	$> 4{,}3 \cdot 10^{23}$ лет	+1	0	0	—
	электронное нейтрино	ν_e	$\tilde{\nu}_e$	$< (2 \div 2{,}5)$ эВ	$\frac{\tau}{m_{\nu_e}} > 300 \frac{c}{\text{эВ}}$	+1	0	0	—
II	мюон	μ^-	μ^+	$\frac{105{,}658}{207{,}767} m_e$	$2{,}197 \cdot 10^{-6}$ с	0	+1	0	$e^- \tilde{\nu}_e \nu_\mu$
	мюонное нейтрино	ν_μ	$\tilde{\nu}_\mu$	< 0,17	$\frac{\tau}{m_{\nu_e}} > 15{,}4 \frac{c}{\text{эВ}}$	0	+1	0	—
III	таон	τ^-	τ^+	1777,0	$0{,}290 \cdot 10^{-12}$ с	0	0	+1	$\mu^- \tilde{\nu}_\mu \nu_\tau$; $e^- \tilde{\nu}_e \nu_\tau$
	таонное нейтрино	ν_τ	$\tilde{\nu}_\tau$	< 18,2	?	0	0	+1	—

Все кварки - фермионы (спин 1/2), с барионным зарядом 1/3. Антикварки имеют квантовые числа с противоположными знаками.

Поколение	Название	Символ	Электр. заряд, ед. e	«Токовая» масса	Проекция изоспина, I_3	Заряд				Блоковая масса (в составе адрона), ГэВ
						c	s	t	b	
I	верхний (up)	u	+ 2/3	1,5—4 МэВ	+ 1/2	0	0	0	0	0,33
	нижний (down)	d	−1/3	4—8 МэВ	−1/2	0	0	0	0	0,33
II	очарованный (charm)	c	+ 2/3	1,1—1,4 ГэВ	0	+ 1	0	0	0	1,8
	странный (strange)	s	−1/3	80—130 МэВ	0	0	−1	0	0	0,51
III	t-кварк (top)	t	+ 2/3	$174{,}3 \pm 5{,}1$ ГэВ	0	0	0	+ 1	0	*)
	b-кварк (bottom)	b	−1/3	4,1—4,4 ГэВ	0	0	0	0	−1	5,0

*) t - кварк имеет такое малое время жизни, что он распадается до образования t - адронов, поэтому блоковой массы не имеет. Токовая масса t - кварка $174{,}3 \pm 5{,}1$ ГэВ.

22.2.7 Estimates in Nuclear Physics

(МК собираю сюда, в 1й части нечего этому делать!)

Оценки ядерных матричных элементов

В сферическом ядре существует вырождение по проекции углового момента с кратностью порядка величины углового момента $l \sim p_{\vec{F}} R$, где R - радиус ядра, а p_F - импульс нуклона на границе ферми. Так как $R = r_0 A^{1/3}$, где r_0-величина порядка среднего расстояния между нуклонами, то $p_F R = p_F r_0 A^{1/3} \sim A^{1/3}$. Следовательно, среднее расстояние между ближайшими уровнями сферического ядра имеет порядок величины $\varepsilon_F / A^{2/3}$.

Оценим сначала расстояние между уровнями, отличающимися лишь радиальными квантовыми числами n, причем $\delta n \sim 1$. Для этого продифференцируем по n условие квантования Бора $\int p_r dr = n$, где p_r - радиальный импульс:

$$1 = \int \frac{\partial p_r}{\partial n} dr = \int \frac{\partial p_r}{\partial \varepsilon_{nl}} \frac{\partial \varepsilon_{nl}}{\partial n} dr \sim \frac{\partial \varepsilon_{nl}}{\partial n} \int \frac{dr}{v} \sim \frac{\partial \varepsilon_{nl}}{\partial n} \frac{R}{v},$$

где ε_{nl}-уровень энергии, а $v = \frac{\partial \varepsilon_{nl}}{\partial p_r}$ - скорость нуклона. В итоге

$$\frac{\partial \varepsilon_{nl}}{\partial n} \sim \frac{v}{R} = \frac{v}{r_0 A^{1/3}} \sim \frac{p_F v}{A^{1/s}} \sim \frac{\varepsilon_F}{A^{1/3}}.$$

22.2.8 Ionizing radiation

(взял из лабника, не будет нужно - уменьшу раздел)

Main methods

Some laboratory examples

(see labnik)

Определение энергии α-частиц по величине их пробега в воздухе

Исследование энергетического спектра β-частиц и определение их максимальной энергии при помощи магнитного спектрометра.

0

Измерение абсолютной активности препарата ^{60}Co методом $\gamma - \gamma$ совпадений

22.2.9 Mass spectrometry

Some laboratory examples

(see labnik)

Измерение коэффициента ослабления потока γ-лучей в веществе и определение их энергии.

Спектрометрия α-излучения с помощь ю полупроводникового детектора.

Определение энергии γ-квантов с помощью сцинтилляционного спектрометра

Исследование процессов взаимодействия γ-излучения со сцинтилляционными детекторами

22.2.10 Structure of Atomic Nuclei

(см. пока ЛЛ3, вообще это отдельное направление, тут основы просто укажу.)

Изотопическая инвариантность

(см. Ландау 3)

Ядерные силы

Оператор взаимодействия двух нуклонов может быть представлен в виде суммы трех (???) независимых членов (?? why??)

$$\widehat{U}_{\text{обыч}} = U_1(r) + U_2(r)\left(\widehat{\mathbf{s}}_1\widehat{\mathbf{s}}_2\right) + U_3(r)\left[3\left(\widehat{\mathbf{s}}_1\mathbf{n}\right)\left(\mathbf{s}_2\mathbf{n}\right) - \widehat{\mathbf{s}}_1\widehat{\mathbf{s}}_2\right]$$

$$\widehat{U}_{\text{обм}} = \left\{U_4(r) + U_5(r)\left(\widehat{\mathbf{s}}_1\widehat{\mathbf{s}}_2\right) + U_6(r)\left[3\left(\widehat{\mathbf{s}}_1\mathbf{n}\right)\left(\widehat{\mathbf{s}}_2\mathbf{n}\right) - \widehat{\mathbf{s}}_1\widehat{\mathbf{s}}_2\right]\right\}\widehat{P}$$

Полный оператор взаимодействия дается суммой

$$\widehat{U} = \widehat{U}_{\text{обыч}} + \widehat{U}_{\text{обм}}\,.$$

при $T = 1 : {}^3P_0^-, {}^3P_1^-, \left({}^3P_2 + {}^3F_2\right)^-, {}^3F_3^-, ...; {}^1S_0^+, {}^1D_2^+, {}^1G_4^+, ...,$
при $T = 0 : \left({}^3S_1 + {}^3D_1\right)^+, {}^3D_2^+ \left({}^3D_3 + {}^3G_3\right)^+, ...; {}^1P_1^-, {}^1F_3^-, ...$

$$R = r_0 A^{1/3},$$

Предельный импульс нуклонов в ядерном веществе.

Объем фазового пространства, соответствующий частицам, находящимся в единице объема физического пространства и обладающим импульсами $p \leqslant p_0$, равен $4\pi p_0^3/3$. Разделив его на $(2\pi\hbar)^3$, получим число «клеток», в каждой из которых может находиться по два протона и два нейтрона. Положив число протонов равным числу нейтронов, получим

$$4\frac{4\pi}{3}\left(\frac{p_0}{2\pi\hbar}\right)^3 = \frac{A}{V}$$

где V - объем ядра. Подставив сюда (117.5), получим

$$p_0 = \left(\frac{3\pi^2 A}{2V}\right)^{1/3}\hbar = \frac{(9\pi)^{1/3}\hbar}{2r_0} = 1,4\cdot 10^{-14}\text{g}\cdot\text{cm}\cdot\text{c}^{-1}.$$

Соответствующая энергия $p_0^2/2m_p$ (m_p - масса нуклона) составляет $\sim$ 30МэВ, а скорость $p_0/m_p \approx c/4$.

Модель оболочек

Для правильного описания, нужно сделать замены: (???)

$$\mathbf{r}_i \to \mathbf{r}_i - \mathbf{R}, \qquad \mathbf{p}_i \to \mathbf{p}_i - \frac{\mathbf{P}}{A}$$

где $\mathbf{R}$ - радиус-вектор центра инерции ядра; A - число частиц в нем; $\mathbf{P}$ - импульс его движения как целого; $\mathbf{p}_i \to \mathbf{p}_i - \frac{\mathbf{P}}{A}$ соответствует вычитанию $\mathbf{v}_i \to \mathbf{v}_i - \mathbf{V}$ из скоростей нуклонов скорости центра инерции $\mathbf{V}$, с которой импульс $\mathbf{P}$ связан соотношением $\mathbf{P} = Am_p\mathbf{V}$ (S. Gartenhaus, C. Schwartz, 1957).

Так, оператор дипольного момента ядра есть $\mathbf{d} = e\sum \mathbf{r}_p$, суммирование производится по всем протонам в ядре. Для вычисления же матричных элементов в методе самосогласованного поля этот оператор надо заменить оператором $e\sum(\mathbf{r}_p - \mathbf{R})$. Координаты центра ядра

$$\mathbf{R} = \frac{1}{A}\left(\sum_p \mathbf{r}_p + \sum_n \mathbf{r}_n\right)$$

Поскольку число протонов в ядре есть Z, то окончательно оператор дипольного момента должен быть заменен согласно

$$e\sum_p \mathbf{r}_p \to e\left(1 - \frac{Z}{A}\right)\sum_p \mathbf{r}_p - e\frac{Z}{A}\sum_n \mathbf{r}_n$$

Из трех векторов $\mathbf{s}, \mathbf{n}$ и $\mathbf{v}$ можно составить истинный скаляр: $[\mathbf{nv}]\mathbf{s}$. Поэтому оператор спин-орбитальной связи нуклона в ядре имеет вид

$$\widehat{V}_{sl} = -\varphi(r)[\mathbf{n}\widehat{\mathbf{v}}]\widehat{\mathbf{s}},$$

где $\varphi(r)$ - некоторая функция от r. Поскольку $m_p[\mathbf{rv}] = \hbar\widehat{\mathbf{l}}$, то

$$\widehat{V}_{sl} = -f(r)\widehat{\mathbf{l}}\widehat{\mathbf{s}},$$

где $f = \hbar\varphi/rm_p$. Подчеркнем, что это взаимодействие-первого порядка по v/c, между тем как спин-орбитальная связь электрона в атоме - эффект второго порядка (§72);

Поскольку

$$\begin{aligned} \mathbf{ls} &= l/2 && \text{при} \quad j = l + 1/2, \\ \mathbf{ls} &= -(l+1)/2 && \text{при} \quad j = l - 1/2 \end{aligned}$$

(по формуле (31.3)), то величина этого расщепления

$$\Delta E = E_{l-1/2} - E_{l+1/2} = \overline{f(r)}(l + 1/2).$$

Следующее правило относится к изотопическому спину ядер. Напомним, что проекция T_ζ изоспина определяется уже весом и номером ядра (см. (116.1)). При заданном значении T_ζ абсолютная величина изоспина может иметь любые значения, удовлетворяющие неравенству $T \gg |T_\zeta|$. Обычно основное состояние ядра имеет наименьшее из этих допустимых значений изоспина, т. е.

$$T_{\text{осн}} = |T_\zeta| = (1/2)(N - Z).$$

Это правило связано с характером взаимодействия нейтрона с протоном, - с тем, что в системе np состояние с изоспином $T = 0$ (состояние нейтрона) имеет бóльшую энергию связи, чем состояние с $T = 1$ (см. примечание на с. 580).

$1s_{1/2}$	2 нуклона,
$1p_{3/2}, 1p_{1/2}$	6 нуклонов,
$1d_{5/2}, 1d_{3/2}, 2s_{1/2}$	12 нуклонов,
$1f_{7/2}, 2p_{3/2}, 1f_{5/2}, 2p_{1/2}, 1g_{9/2}$	30 нуклонов,
$2d_{5/2}, 1g_{7/2}, 1h_{11/2}, 2d_{3/4}, 3s_{1/2}$	32 нуклона,
$2f_{7/2}, 1h_{9/2}, 1i_{13/2}, 2f_{5/2}, 3p_{3/2}, 3p_{1/2}$	44 нуклона.

Для каждой группы указано полное число протонных или нейтронных вакансий. Соответственно этим числам заполнение какой-либо из групп заканчивается, когда полное число протонов Z или нейтронов N в ядре равно одному из следующих чисел:

$$2, 8, 20, 50, 82, 126.$$

Эти числа принято называть магическими.

$$\widehat{\overline{\boldsymbol{\mu}}} = \mu_0 g \widehat{\mathbf{J}}$$

где μ_0 - ядерный магнетон, а g-гиромагнитный множитель. Собственное значение проекции этого момента $\bar{\mu}_z = \mu_0 g M_J$. Обычно (ср. (111.1)) под магнитным моментом μ, ядра понимают просто максимальное значение его проекции, т. е. $\mu = \mu_0 g J$; с таким обозначением

$$\widehat{\overline{\boldsymbol{\mu}}} = \mu(\widehat{\mathbf{J}}/J).$$

С указанными выше значениями гиромагнитных множителей это дает для магнитного момента протона $\mu_p = g_j j$:

$$\begin{aligned} \mu_p &= \left(1 - \tfrac{2{,}29}{j+1}\right) j \quad \text{при} \quad j = l - 1/2, \\ \mu_p &= j + 2{,}29 \quad \text{при} \quad j = l + 1/2 \end{aligned}$$

и для магнитного момента нейтрона

$$\begin{aligned} \mu_n &= \tfrac{1{,}91}{j+1} j \quad \text{при} \quad j = l - 1/2. \\ \mu_n &= -1{,}91 \quad \text{при} \quad j = l + 1/2 \end{aligned}$$

$$\varphi(r)\frac{e}{cm_p}[\mathbf{nA}]\widehat{\mathbf{s}} = f(r)\frac{e}{2c\hbar}[\mathbf{r}[\mathbf{Hr}]]\widehat{\mathbf{s}} = f(r)\frac{e}{2c\hbar}[\mathbf{r}[\widehat{\mathbf{s}}\mathbf{r}]\mathbf{H}$$

Такой член эквивалентен возникновению дополнительного магнитного момента с оператором

$$\widehat{\mu}_{\text{доп}} = -\frac{e}{2c\hbar} f(r)[\mathbf{r}[\widehat{\mathbf{s}}\mathbf{r}]] = -\frac{e}{2c\hbar} r^2 f(r)\{\widehat{\mathbf{s}} - (\widehat{\mathbf{s}}\mathbf{n})\mathbf{n}\}.$$

Несферические ядра

Полный момент вращающегося ядра $\mathbf{J}$, разумеется, сохраняется. При заданном Ω его величина J пробегает значения, начинающиеся от Ω:

$$J = \Omega, \quad \Omega + 1, \quad \Omega + 2, \ldots$$

(см. (83.2)). Дополнительное ограничение возможных значений J имеет место для ядер с $\Omega = 0$: в состояниях 0_g^+ и 0_u^- число J пробегает лишь четные значения, а в состояниях 0_g^- и 0_u^+- нечетные (см. §86). В частности, во вращательных уровнях основного терма четно-четных ядер $\left(0_g^+\right)$ число J пробегает значения $0, 2, 4, \ldots$ Вращательная энергия ядра определяется формулой

$$E_{\text{Вр}} = \frac{\hbar^2}{2I} J(J+1)$$

Как известно из механики (см. I, §39), энергия частицы во вращающейся системе координат содержит дополнительный член, равный произведению угловой скорости вращения на момент импульса частицы. Соответствующий член в гамильтониане ядра можно представить в виде $2b\widehat{\mathbf{K}}\widehat{\boldsymbol{\sigma}}$, где b-некоторая постоянная; $\widehat{\mathbf{K}}$ - вращательный момент остова ядра (ядро без последнего нуклона), а $\widehat{\boldsymbol{\sigma}}$ - момент нуклона; последний надо понимать здесь в чисто формальном смысле (в действительности вектор момента нуклона в аксиальном поле ядра не существует), как оператор, аналогичный оператору спина $1/2$, дающий переходы между состояниями со значениями проекции момента $\pm 1/2$ - в соответствии со значением $\Omega = 1/2$[1]). Поскольку $\mathbf{K} = \mathbf{J} - \boldsymbol{\sigma}$, то собственные значения этого оператора

$$2b\mathbf{K}\boldsymbol{\sigma} = b\left[J(J+1) - K(K+1) - \frac{3}{4}\right].$$

Добавив сюда для удобства не зависящую от J постоянную $b/2$, найдем, что эта величина равна $\pm b(J+1/2)$ при $J = K \pm 1/2$. Это выражение можно записать в виде $(-1)^{J-1/2}b(J+1/2)$, если учесть, что момент K остова (представляющего собой четно-четное ядро) является четным числом. Таким образом,

окончательно получаем следующее выражение для вращательной энергии ядра с $\Omega = 1/2$:

$$E_{\text{Вр}} = \frac{\hbar^2}{2I}J(J+1) + (-1)^{J-1/2}b\left(J + \frac{1}{2}\right)$$

(A. Bohr, B. Mottelson, 1953). Отметим, что если постоянная b положительна и достаточно велика, то уровень с $J = 3/2$ может оказаться лежащим ниже уровня с $J = 1/2$, т.е. может нарушиться нормальный порядок вращательных уровней, при котором низший уровень соответствует наименьшему возможному значению J.

$$\boldsymbol{\mu} = \mu'\mathbf{n} + g_r(\mathbf{J} - \Omega\mathbf{n}).$$

Здесь g_r есть гиромагнитный множитель вращения ядра. Поскольку вклад в магнитный момент при вращении дают только протоны, то

$$g_r = \frac{I_p}{I_p + I_n}$$

где I_n и I_p - нейтронная и протонная части момента инерции ядра (для системы из одних только протонов должно было бы быть просто $g_r = 1$). Отношение (119.5), вообще говоря, не совпадает с отношением Z/A числа протонов к полной массе ядра.

После усреднения по вращению ядра магнитный момент направлен по сохраняющемуся вектору $\mathbf{J}$:

$$\overline{\widehat{\boldsymbol{\mu}}} = \frac{\mu}{J}\widehat{\mathbf{J}} = (\mu' - \Omega g_r)\,\overline{\mathbf{n}} + g_r\widehat{\mathbf{J}}.$$

Как обычно, умножаем обе части этого равенства на $\widehat{\mathbf{J}}$ и переходим к собственным значениям. В основном состоянии ядра $\Omega = J$ в результате находим

$$\mu = (\mu' + g_r)\,\frac{J}{J+1}.$$

Изотопическое смещение

У двух изотопов (одинаковых элементов, но с разным числом протонов и нейтронов в ядре) разная энергия, она равна разности энергий

$$E = \frac{2\pi}{3}\psi^2(0)Ze^2\overline{r^2}$$

Тут $\overline{r^2} = \frac{1}{Ze}\int \rho r^2 dV$ - протонный средний квадратичный радиус ядра (при однородном распределении протонов $\overline{r^2} = 3R^2/5$, где R - геометрический радиус ядра).

Обоснование следующее. В легких атомах основным источником изотопического смещения является эффект конечности массы ядра. $\frac{1}{2M}\left(\sum_i \widehat{\mathbf{p}}_i\right)^2$, где M - масса ядра, а $\mathbf{p}_i$ - импульсы электронов. Поэтому связанное с данным эффектом изотопическое смещение находится как среднее значение $\frac{1}{2}\left(\frac{1}{M_1}-\frac{1}{M_2}\right)\overline{\left(\sum_i \mathbf{p}_i\right)^2}$, вычисленное по волновой функции данного состояния атома (M_1, M_2 - массы ядер изотопов).

$$\Delta E = -e\int\left(\varphi - \frac{Ze}{r}\right)\psi^2(r)dV = \overset{\Delta r^2=6}{=} -\frac{1}{6}e\psi^2(0)\int\left(\varphi-\frac{Ze}{r}\right)\Delta r^2 dV = -\frac{1}{6}e\psi^2(0)\int r^2\Delta\left(\varphi-\frac{Ze}{r}\right)dV$$

(??? подумаю еще про это!) Тут $\Delta\frac{1}{r} = -4\pi\delta(\mathbf{r})$, а $r^2\delta(\mathbf{r}) = 0$ при всех r. Также по уравнению Пуассона $\Delta\varphi = -4\pi\rho$, где ρ - плотность распределения электрического заряда в ядре. Отсюда и заявленная формула.

В §71ЛЛ3 была произведена оценка величины $\psi(0)$ и выяснено, что она зависит от (предполагаемого большим) атомного номера как $\sqrt{Z}$. Поэтому величина расщепления (120.3) оказывается пропорциональной R^2Z^2.

Об учете движения ядра (???)

(??? как это учесть??? тоже от этого поправка есть какая-то???)

22.2.11 Hyperfine Structure (!?)

(пока только тут про это планирую писать, чуть что - отдельная запись.)

Основные свойства

(напишу когда-то суть, типа такие-то вклады, квадрупольное, магнитодипольное, да???)

Hyperfine structure comes from the multipole moments of the atomic nucleus, in particular the magnetic dipole and electric quadrupole fields.

- Hyperfine effects couple the nucleus and electrons together, thereby enlarging the Hilbert space. They have many useful applications. For example, the hyperfine splitting of the ground state of hydrogen produces the 21 cm line, which is useful in radio astronomy. Most atomic clocks use the frequency of a hyperfine transition in a heavy alkali atom, such as rubidium or cesium, the latter of which defines the second.

- We will denote the spin of the nucleus by $\mathbf{I}$, and as usual assume the nucleus is described by a single irrep, of I^2 eigenvalue $i(i+1)\hbar^2$. The nucleus Hilbert space is spanned by $|im_i\rangle$.

- For stable nuclei, i ranges from 0 to 15/2. For example, the proton has $i = 1/2$, the deuteron has $i = 1$, and ^{133}Cs, used in atomic clocks, has $i = 7/2$.

- We restrict to nuclei with $i = 1/2$, in which case the only possible multipole moment, besides the electric monopole, is the magnetic dipole.

Expansion of the Hamiltonian and terms for hyperfine structure

$$\mathbf{A}(\mathbf{r}) = (\boldsymbol{\mu} \times \mathbf{r}) \left(\frac{4\pi}{3} \delta(\mathbf{r}) + \frac{1}{r^3} \right), \qquad \mathbf{B}(\mathbf{r}) = \boldsymbol{\mu} \cdot \left(\frac{8\pi}{3} \delta(\mathbf{r}) I + \frac{T}{r^5} \right). \text{ (dipole)}$$

Here we're mixing vector and tensor notation; I is the identity tensor, T is the quadrupole tensor, and dotting with $\boldsymbol{\mu}$ on the left indicates contraction with the first index. The delta function terms, present for all physical dipoles, will be important for the final result.

- The Hamiltonian is similar to that of the Zeeman effect,

$$H = \frac{1}{2} \left(\mathbf{p} + \frac{\mathbf{A}}{c} \right)^2 + V(r) + H_{\text{FS}} + H_{\text{Lamb}} + \frac{1}{c} \mathbf{S} \cdot \mathbf{B}.$$

The magnetic moment of the nucleus is

$$\boldsymbol{\mu} = g_N \mu_N \mathbf{I}$$

where μ_N is the nuclear magneton. The states in the Hilbert space can be written as $|n\ell j m_j m_i\rangle$, which we refer to as the "uncoupled" basis since $\mathbf{J}$ and $\mathbf{I}$ are uncoupled.

- As in our analysis of the Zeeman effect, the vector potential is in Coulomb gauge and the A^2 term is negligible, so by the same logic we have

$$H_1 = \frac{1}{c} (\mathbf{p} \cdot \mathbf{A} + \mathbf{S} \cdot \mathbf{B}).$$

However, it will be more difficult to evaluate these orbital and spin terms.

- The orbital term is proportional to

$$\mathbf{P} \cdot (\mathbf{I} \times \mathbf{r}) = \mathbf{I} \cdot (\mathbf{r} \times \mathbf{p}) = \mathbf{I} \cdot \mathbf{L}$$

where one can check there are no ordering issues. Similarly, there are no ordering issues in the spin term, since $\mathbf{S}$ and $\mathbf{I}$ act on separate spaces. Hence we arrive at

$$H_{1,\text{orb}} = k(\mathbf{I} \cdot \mathbf{L}) \left(\frac{4\pi}{3} \delta(\mathbf{r}) + \frac{1}{r^3} \right), \quad H_{1,\text{spin}} = k \left(\frac{8\pi}{3} \delta(\mathbf{r}) (\mathbf{I} \cdot \mathbf{S}) + \frac{\mathbf{I} \cdot T \cdot \mathbf{S}}{r^5} \right).$$

The delta function terms are called Fermi contact terms, and we have defined

$$k = 2 g_N \mu_B \mu_N = g_e g_N \mu_B \mu_N.$$

The term $H_{1,\text{ spin}}$ is a spin-spin interaction, while $H_{1,\text{ orb}}$ can be thought of as the interaction of the moving electron with the proton's magnetic field.

- It's tempting to add in additional terms, representing the interaction of the proton's magnetic moment with the magnetic field produced by the electron, due to its spin and orbital motion. These give additional copies of $H_{1,\text{ spin}}$ and $H_{1,\text{ orb}}$ respectively, but they shouldn't be added since they would double count the interaction.

- The terms I - L and I - S don't commute with $\mathbf{L}, \mathbf{S}$, or $\mathbf{I}$. So just as for fine structure, we are motivated to go to the coupled basis. We define $\mathbf{F} = \mathbf{J} + \mathbf{I}$ and diagonalize L^2, J^2, F^2, and F_z. The coupled basis is related to the uncoupled one as

$$|n\ell j f m_f\rangle = \sum_{m_j, m_i} |n\ell j m_j m_i\rangle \langle j i m_j m_i | f m_f\rangle .$$

To relate this coupled basis to the original uncoupled basis $|n\ell m_\ell m_s m_f\rangle$, we need to apply Clebsch-Gordan coefficients twice. Alternatively, we can use tools such as the Wigner 6j symbols or the Racah coefficients to do the addition in one step.

Calculation of the energy shifts for hyperfine structure

- In the coupled basis, the perturbation is diagonal, so we again can avoid diagonalizing matrices. It suffices to compute diagonal matrix elements,

$$\Delta E = \langle n\ell jfm_f \left|H_1\right| n\ell jfm_f\rangle$$

- First we consider the case $\ell \neq 0$, where the contact terms do not contribute. We can write the energy shift as

$$\Delta E = k \langle n\ell jfm_f|\mathbf{I}\cdot\mathbf{G}|n\ell jfm_f\rangle\,, \quad \mathbf{G} = \frac{\mathbf{L}}{r^3} + \frac{T\cdot\mathbf{S}}{r^5} = \frac{\mathbf{L}}{r^3} + \frac{3\mathbf{r}(\mathbf{r}\cdot\mathbf{S}) - r^2\mathbf{S}}{r^5}.$$

- The quantity $\mathbf{G}$ is a purely electronic vector operator, and we are taking matrix elements within a single irrep of electronic rotations (generated by $\mathbf{J}$), so we may apply the projection theorem,

$$\Delta E = \frac{k}{j(j+1)} \langle n\ell jfm_f|(\mathbf{I}\cdot\mathbf{J})(\mathbf{J}\cdot\mathbf{G})|n\ell jfm_f\rangle\,.$$

- The first term may be simplified by noting that

$$\mathbf{I}\cdot\mathbf{J} = \frac{1}{2}\left(F^2 - J^2 - I^2\right).$$

This gives a factor similar to the Lande g-factor.

- For the second term, direct substitution gives

$$\mathbf{J}\cdot\mathbf{G} = \frac{L^2 - S^2}{r^3} + \frac{3(\mathbf{r}\cdot\mathbf{S})^2}{r^5}$$

where we used $\mathbf{r}\cdot\mathbf{L} = 0$. Now, we have

$$(\mathbf{r}\cdot\mathbf{S})^2 = \frac{1}{4}r_i r_j \sigma_i \sigma_j = \frac{1}{4}r_i r_j \left(\delta_{ij} + i\epsilon_{ijk}\sigma_k\right) = \frac{r^2}{4}.$$

Plugging this in cancels the $-S^2/r^3$ term, leaving

$$\mathbf{J}\cdot\mathbf{G} = \frac{L^2}{r^3}.$$

- Therefore, the energy shift becomes

$$\Delta E = k\frac{f(f+1) - j(j+1) - i(i+1)}{2j(j+1)}\ell(\ell+1)\left\langle\frac{1}{r^3}\right\rangle.$$

Specializing to hydrogen and evaluating $\langle 1/r^3\rangle$ as earlier, we get the final result

$$\Delta E = \frac{g_e g_N \mu_B \mu_N}{a_0^3}\frac{1}{n^3}\frac{f(f+1) - j(j+1) - i(i+1)}{j(j+1)(2\ell+1)}$$

where we restored the Bohr radius.

- Now consider the case $\ell = 0$. As we just saw, the non-contact terms get a factor of $\mathbf{J}\cdot\mathbf{G} = L^2/r^3$, so they vanish in this case. Only the contact term in $H_{1,\,\text{spin}}$ contributes, giving

$$\Delta E = \frac{8\pi}{3}k\langle\delta(\mathbf{r})(\mathbf{I}\cdot\mathbf{S})\rangle.$$

Since $\mathbf{F} = \mathbf{I} + \mathbf{S}$ when $\mathbf{L} = 0$, we have

$$\mathbf{I} \cdot \mathbf{S} = \frac{1}{2}\left(F^2 - I^2 - S^2\right) = \frac{1}{2}\left(f(f+1) - \frac{3}{2}\right).$$

The delta function is evaluated as for the Darwin term. The end result is that the energy shift we found above for $\ell \neq 0$ also holds for $\ell = 0$.

- When the hyperfine splitting is included, the energy levels become $E_{n\ell jf}$. The states $|n\ell jfm_f\rangle$ are $(2f+1)$-fold degenerate.

- For example, the ground state $1s_{1/2}$ of hydrogen splits into two levels, where $f = 0$ is the true ground state and $f = 1$ is three-fold degenerate; these correspond to antiparallel and parallel nuclear and electronic spins. The frequency difference is about 1.42GHz, which corresponds to a 21 cm wavelength.

- The $2s_{1/2}$ and $2p_{1/2}$ states each split similarly; the hyperfine splitting within these levels is smaller than, but comparable to, the Lamb shift between them. The fine structure level $2p_{3/2}$ also splits, into $f = 1$ and $f = 2$.

- Electric dipole transitions are governed by the matrix element

$$\left\langle n\ell jfm_f \left| x_q \right| n'\ell' j' f' m_f' \right\rangle.$$

The Wigner-Eckart theorem can be applied to rotations in $\mathbf{J}, \mathbf{F}$, and I separately, under each of which x_q is a $k = 1$ irreducible tensor operator, giving the constraints

$$m_f = m_f' + q, \quad |\Delta f| \leq 1, \quad |\Delta j| \leq 1, \quad |\Delta \ell| \leq 1.$$

As usual, parity gives the additional constraint $\Delta\ell \neq 0$.

- Finally, there is a special case for $f' = 0$, because this is the only representation that, upon multiplication by the spin 1 representation, does not contain itself: $0 \notin 0 \otimes 1$. This means we cannot have a transition from $f' = 0$ to $f = 0$. The same goes for ℓ, but this case is already excluded by parity.

- Note that the 21 cm line of hydrogen is forbidden by the rules above; it actually proceeds as a magnetic dipole transition. The splitting is small enough for it to be excited by even the cosmic microwave background radiation. The 21 cm line is especially useful because its wavelength is too large to be scattered effectively by dust. Measuring its intensity gives a map of the atomic hydrogen gas distribution, measuring its Doppler shift gives information about the gas velocity, and measuring its line width determines the temperature. Doppler shift measurements were used to map out the arms of the Milky Way. (These statements hold for atomic hydrogen; molecular hydrogen (H_2) has a rather different hyperfine structure.)

- It is occasionally useful to consider both the weak-field Zeeman effect and hyperfine structure. Consider a fine structure energy level with $j = 1/2$. For each value of m_f there are two states, with $f = i \pm 1/2$. The two perturbations don't change m_f, so they only mix pairs of states. Thus the energy level splits into pairs of levels, which are relatively easy to calculate; the result is the Breit-Rabi formula. The situation is just like how the Zeeman effect interacts with fine structure, but with (ℓ, s) replaced with (j, i). At lower fields the coupled basis is preferred, while at higher fields the uncoupled basis is preferred.

Сверхтонкая структура атомных уровней

(?????? вот тут у Ландау мб фигня, потом про это нужно еще думать много)

та. По общим правилам сложения моментов квантовое число F принимает значения

$$F = J + i, \quad J + i - 1, ..., |J - i|,$$

так что каждый уровень с заданным J расщепляется на $2i+1$ (если $i<J$) или $2J+1$(если $i>J$) компонент.

Поскольку средние расстояния r электронов в атоме велики по сравнению с радиусом R ядра, основную роль в сверхтонком расщеплении играет взаимодействие электронов с мультипольными моментами ядра наиболее низких порядков. Таковыми являются магнитный дипольный и электрический квадрупольный моменты (средний дипольный момент равен нулю-см. 75). Магнитный момент ядра имеет порядок величины $\mu_{\text{яд}} \sim \sim eRv_{\text{яд}}/c$, где $v_{\text{яд}}$ - скорости нуклонов в ядре. Энергия его взаимодействия с магнитным моментом электрона ($\mu_{\text{эл}} \sim e\hbar/mc$)

порядка

$$\frac{\mu_{\text{Яд}}\,\mu_{\text{эл}}}{r^3} \sim \frac{e^2\hbar}{mc^2}\frac{Rv_{\text{яд}}}{r^3}.$$

Квадрупольный момент ядра $Q \sim eR^2$; энергия взаимодействия создаваемого им поля с зарядом электрона порядка

$$\frac{eQ}{r^3} \sim \frac{e^2R^2}{r^3}.$$

Сравнивая (121.2) и (121.3), мы видим, что магнитное взаимодействие (а потому и вызываемое им расщепление уровней) в $(v_{\text{яд}}/c)\,(\hbar/mcR) \sim 15$ раз больше квадрупольного взаимодействия; хотя отношение $v_{\text{яд}}/c$ сравнительно мало, зато отношение $\hbar/mcR$ велико.

Оператор магнитного взаимодействия электронов с ядром имеет вид

$$\widehat{V}_{iJ} = a\widehat{\mathbf{i}}\widehat{\mathbf{J}}$$

(аналогично спин-орбитальному взаимодействию электронов (72.4)). Зависимость вызываемого им расщепления уровней от F дается, следовательно, выражением

$$\frac{a}{2}F(F+1)$$

Согласно известной формуле электродинамики это поле

$$\widehat{\mathbf{H}} = \frac{1}{c}\int \frac{[\widehat{\mathbf{n}}]}{r^2}dV,$$

где $\hat{\mathbf{j}}$ - оператор плотности тока, создаваемого движущимся электронным спином, а $\mathbf{r}=\mathbf{n}r$-радиус-вектор из центра К элементу dV[2]). Согласно (115.4) имеем

$$\widehat{\mathbf{j}} = -2\mu_B c\,\mathrm{rot}\left(\psi^2\widehat{\mathbf{s}}\right) = -2\mu_B c\frac{d\psi^2(r)}{dr}[\mathbf{n}\widehat{\mathbf{s}}]$$

)μ_B - магнетон Бора). Написав $dV=r^2drdo$ и произведя интегрирование, находим

$$\widehat{\mathbf{H}} = -2\mu_B\int_0^\infty \frac{d\psi^2}{dr}dr\int[\mathbf{n}[\mathbf{n}\widehat{\mathbf{s}}]]do = -2\mu_B\psi^2(0)\frac{8\pi}{3}\widehat{\mathbf{s}}.$$

Окончательно для оператора взаимодействия имеем

$$\widehat{V}_{is} = -\widehat{\boldsymbol{\mu}}\widehat{\mathbf{H}} = \frac{16\pi}{3i}\mu\mu_B\psi^2(0)\widehat{\mathbf{i}}\widehat{\mathbf{s}}.$$

$$E_{i+1/2} - E_{i-1/2} = \frac{8\pi}{3i}\mu\mu_B(2i+1)\psi^2(0)$$

Сверхтонкая структура молекулярных уровней (????)

(???? это заново читать нужно, пока не усвоено и не актуально)

Для $\widehat{Q}_{ii}=0$: (??? о чем речь???)

$$\widehat{b}\widehat{i}_i\widehat{i}_k\left(n_in_k-\frac{1}{3}\delta_{ik}\right)$$

при заданной величине проекции i_ζ спина ядра на ось молекулы эта величина равна $b\left[i_\zeta^2-\frac{1}{3}i(i+1)\right]$.

В результате же усреднения оператора (122.1) по вращению молекулы он оказывается выраженным через оператор $\widehat{\mathbf{K}}$ сохраняющегося вращательного момента. Усреднение произведения n_in_k производится по формуле, полученной в задаче к §29 (с вектором $\mathbf{K}$ вместо 1), и дает в результате

$$-\frac{b}{(2K-1)(2K+3)}\widehat{i}_i\widehat{i}_k\left[\widehat{K}_i\widehat{K}_k+\widehat{K}_k\widehat{K}_i-\frac{2}{3}\delta_{ik}K(K+1)\right].$$

Собственные значения этого оператора находятся так же, как это было указано для оператора (121.6).

В случае многоатомной молекулы вместо (122.1) получается, вообще говоря, оператор вида

$$b_{ik}\widehat{i}_i\widehat{i}_k$$

$$\overline{J_\zeta^2}=k^2,\overline{J_\xi^2}=\overline{J_\eta^2}=\frac{1}{2}\left[J(J+1)-k^2\right].$$

Если спины ядер равны $1/2$, квадрупольное взаимодействие отсутствует.

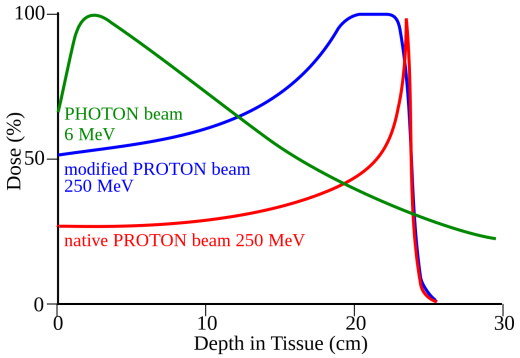
Одним из основных источников сверхтонкого расщепления в этом случае является прямое магнитное взаимодействие ядерных магнитных моментов друг с другом. Оператор взаимодействия двух магнитных моментов $\boldsymbol{\mu}_1=\mu_1\mathbf{i}_1/i_1,\boldsymbol{\mu}_2=\mu_2\mathbf{i}_2/i_2$ дается формулой

$$\frac{\mu_1\mu_2}{i_1i_2r^3}\left[\widehat{\mathbf{i}}_1\widehat{\mathbf{i}}_2-3\left(\mathbf{i}_1\mathbf{n}\right)\left(\mathbf{i}_2\mathbf{n}\right)\right]$$

22.3 Other Quantum Phenomena

22.3.1 Penetration of particles through medium in a nutshell

Bragg peaks and etc



(??? a paragraph about treating cancer with protons. Why exactly this way it is possible to do it? also I'll add some important formulas)

(пока у меня в ЭД сплошных сред это, потому что Ландау про это там написал. Все равно, специфическая тема, можно и не знать ее и жить счастливо)

22.3.2 Cosmic rays

(see labnik 5 semestr)

Cosmic rays experiments

22.3.3 Magnetic resonances and nuclei

(see labnik 5 semestr)

Общая теория магнитного резонанса

Магнитный резонанс - это избирательное поглощение веществом электромагнитных волн определенной частоты, обусловленное изменением ориентации магнитных моментов частиц вещества. Если поглощение энергии осуществляется ядрами, то магнитный резонанс называется ядерным магнитным резонансом (ЯМР). Магнитный резонанс, обусловленный магнитными моментами неспаренных электронов в парамагнетиках, называется электронным парамагнитным резонансом (ЭПР). В магнитоупорядоченных веществах электронный магнитный резонанс называют антиферромагнитным или ферромагнитным в зависимости от симметрии упорядочения.

(см первые страницы раздела X лабника про это)

Электронный парамагнитный резонанс (ЭПР)

Классическая интерпретация этих резонансный явлений следующая. У нас есть спин (в случае электронного парамагнитного резонанса у электрона, в случае ядерного - у ядра), у нас есть внешнее постоянное магнитное поле. Спин может быть направлен по или против этого поля, в зависимости от этого энергия у такого спина будет разной. Но под действием внешнего переменного поля мы можем заставить спин поворачиваться. Это соответствует обычному переходу в двухуровневой системе. В качестве альтернативы, можно сказать, что это переход соответствует $M1$ фотонам.

Основная формула этого эффекта:

$$\hbar\omega_0 = g\mu B$$

(?? видимо, лабник нужно читать еще много!)

Сверхтонкая структура электронного парамагнитного резонанса

Изучение ядерного магнитного резонанса (ЯМР)

(!! тут важный абзац с сутью явления!)

$$E = -(\boldsymbol{\mu}, \mathrm{B})$$

$$\mu = \gamma \mathrm{M}$$

$$\mu_\mathrm{s} = \frac{e\hbar}{2m_p} = 0,5 \cdot 10^{-23} \cdot \text{ c}^{-1}$$

$$g = \frac{\mu/\mu_\mathrm{g}}{M/\hbar} = \frac{\mu}{\mu_\mathrm{g}}\frac{\hbar}{M} = \frac{\hbar}{\mu_\mathrm{g}}\gamma.$$

$$\boldsymbol{\mu} = \frac{\mu_\mathrm{g}}{\hbar} g \mathrm{M}$$

$$\mathrm{M}^2 = \hbar^2 I(I+1)$$

$$M_z = m\hbar$$

$$-I \leqslant m \leqslant +I$$

$$\mu_B = \frac{\mu_\mathrm{g}}{\hbar} g M_B = \frac{\mu_\mathrm{g}}{\hbar} g m \hbar = \mu_\mathrm{g} g m.$$

$$\Delta E = B \Delta \mu_B = B \mu_\mathrm{q} g \Delta m = B \mu_\mathrm{q} g.$$

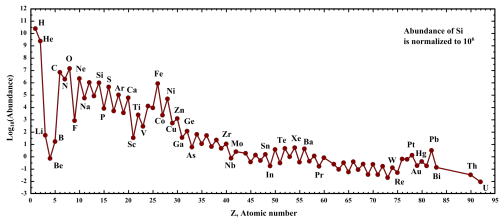
(вставлю картинку из лабника!)
(потом еще пара страниц теории)

Магнитные моменты легких ядер

22.3.4 Stars, atoms a Universe

(связь с астрофизикой и космологией, там это подробнее написано. интересные модели, додумаю потом.)

Properties of a solar system that are described by QM



Суть источников излучения звезд

(потом допишу)

Суть анализа нейтронных звезд на устойчивость

Примеры квантовых свойств звезд и планет

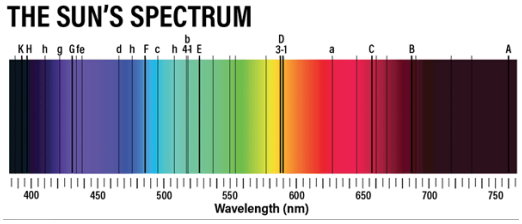
О солнце

Hydrogen and helium are by far the most abundant elements found in the Sun, making up about 98 percent of its mass, but other, heavier elements play an important role in the physical processes that occur in the Sun. The process of nuclear fusion combines hydrogen atoms to produce helium and the energy that keeps the Sun shining.

he next three elements heavier than helium — lithium, beryllium, and boron — are sometimes formed as intermediate products during the fusion process. Elements even heavier than these are present throughout the Sun. They come not from nuclear fusion in our own Sun, but from previous generations of massive stars in the solar neighborhood, the remains of which have been scattered by supernova explosions. The same cloud of enriched material that formed the Sun also formed Earth and the other planets. Thus, the same naturally occurring elements that

can be found on Earth, up to and including elements as heavy as uranium, are also present in the Sun.

Although elements heavier than helium are much less common than hydrogen and helium in the Sun, elements like iron, nickel, calcium, sodium, and magnesium are prominent in the solar spectrum and are important tools for astronomers studying the Sun.



(это не полностью еще понимаю, додумаю потом когда-то, тут больше объема про Солнце не планирую.)

О фотонах в космологии

(пока об этом в космологии)

Atoms in an Expanding Universe by Tong

(пара страниц у него про это, интересно, но не до этого)

Quantum mechanics for Black holes

(пока в записи по гравитации, но потом сюда добавлю. см. пока задачу Киселева про квазиклассику и черную дыру)

22.4 Modifications and Generalizations of QM

22.4.1 SUSY QM (???)

Суть

(пока не касался, мб потом займусь, пока нет таких планов)

Примеры применения (??)

(пока не касался, мб потом займусь, пока нет таких планов)

22.4.2 QFT as a generalization of QM (???)

22.4.3 Review of Other Theoretical Modifications of QM

О p-адической квантовой механике и других полях чисел (???)

(есть статьи, когда-то мб почитаю, пока не до них)

Какую по итогу роль играют поля чисел в квантмехе (???)

(не знаю и мне минимум неделя уйдет понять это.)

Part VII
Introduction to Other Parts of QM

23 Experiments in Quantum Mechanics

Обсудим различные эксперименты в квантовой механике.

(??? уже где-то должен был быть этот раздел, если его не было, то тут будет. странно, что так не находится сразу он. такой вот подглавы должно хватить, итак много места указать многое.)

23.1 Review of Basic Devices for Experiments in QM

Обсудим различные квантовые приборы.

!!! по сути мы уже все это прошли, особенно когда делали лабы - все это изучали. особенно в оптике кстати.

просто потом придет отдельное время - я внимательно посмотрю на приборы, что они показывают и как работают.

это важный, но второстепенный раздел.

актуальные квантовые приборы

Обсудим сперва самые полезные квантовые приборы.

камера Вильсона

самый интересный прибор будто бы.

лабораторные приборы

монохроматоры

полезные вещи, на лабах они везде, потом разберу, что можно с ними интересного сказать про физику.

опыты!!!

осциллограф

я знаю, что это в электричестве, но пока буду писать сюда.

приборы для физики элементарных частиц

газовые детекторы

полупроводниковые детекторы

калориметры

23.2 How Exactly Basic Experiments of Quantum Mechanics Were Made?

(мб в другое место это напишу, пока тут. скорее не задачи, а просто каталог моделей)

23.2.1 Photoelectric Effect

(тут вмеру подробно обсуждаю, подробнее - только КТП.)

Суть фотоэффекта

Суть в том, что при облучении металлов светом определенной волны, из этих металлов могут выбиваться электроны.

Соотношение между энергией падающего фотона, работой выхода и кинетической энергией электронов есть

$$E_{h\nu} = A + T_e$$

Идейные вопросы о фотоэффекте

(тут полно их будет...)

Нормальная модель и описание фотоэффекта

тут КТП

Упрощенная модель фотоэффекта

(общефиз)

фотоэффект

Фотоэффект - испускание электронов фотокатодом, облучаемым светом (любым что ли, который выбьет частицы?)

Рассматривается катод (про другие материалы - хз), на который падает фотон $\hbar\omega$.

Энергетический баланс описывается *уравнением Эйнштейна*:

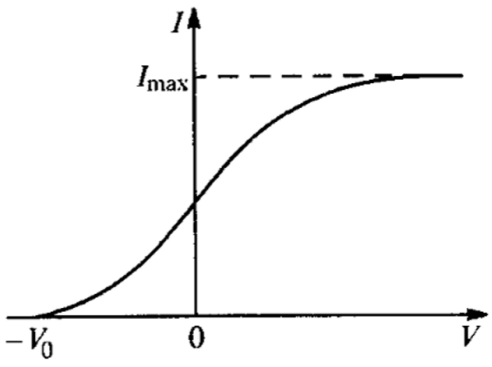
$$\hbar\omega = E_{\max} + A_{\text{вых}}$$

(возможно, наше внимание тут обращают на то, что энергия почти всегда меньше максимальной, а это уравнение справедливо только для максимальной?)

мы хотим измерять энергию вылетевших электронов вблизи катода.

для этого поместим анод рядом с ним и на него будем подавать разные потенциалы, а также измерять ток через него.

ток на аноде имеет такую зависимость для данной частоты фотонов:



В таком случае если мы приложим положительный потенциал V, то все выбитые фотоэлектроны достигнут анода, а если подадим задерживающее напряжение - то какие-то, которые с меньшей энергией вылетели, не смогут достичь анода, а при уменьшении

напряжения настанет случай, когда только с максимальной энергией электроны смогут достигать анод, этот потенциал называется *потенциал запирания* V_0. (в реальности есть какая-то оговорка про это, что сложно его поменять)

поэтому при потенциале запирания $E_{max} = eV_0$.

таким образом, зная работу выхода, зависимость запирающего потенциала от частоты имеет вид $eV_0 = \hbar\omega - W$.

окей, теперь в реальности оказывается, что выбиваются электроны не только с самых поверхностей материала, а еще и из внутренних частей, поэтому (я хз, ка это связано на самом деле, но так говорят) поэтому наблюдается плавное уменьшение фототока.

Чтобы определить зависимость тока от задерживающего потенциала, построим модель вылетающих электронов, распределенных по гауссу:

$$n(\vartheta) = n_0 e^{-\delta^2/\hat{v}_0^2}$$

,

где v_0 - ширина углового распредееления.

Тогда

$$dn(\vartheta) = n(\vartheta)d\vartheta = 2\pi n_0 \sin\vartheta e^{-j^2/D_0^2} d\vartheta$$

(я хз, откуда 2π, все заметаем под ковер словами "так расписывается телесный угол)

а так как фототок при малых углах будет, то нужно рассмотреть

$$dn(\vartheta) \simeq 2\pi n_0 \vartheta \left(1 - \vartheta^2/\overline{\vartheta}_0^2\right) d\vartheta$$

Ток I, или число электронов за единицу веремени, под углами меньшими θ определяется

$$N(\vartheta) = 2\pi n_0 \int_0^{\mathfrak{d}} \vartheta \left(1 - \mathfrak{v}^2/\overline{\vartheta}_0^2\right) d\vartheta = 2\pi n_0 \left(\vartheta^2/2 - \vartheta^4/4\overline{\vartheta_0^2}\right)$$

критический угол определяется из энергий, при угле большем скорости тупо не хватит: θ: $V = mv_z^2/2 = mv_0^2 \cos^2\vartheta/2$, расписывая cos для малого угла и вводя V_0, видим зависимость максимального угла отклонения от напряжения:$\vartheta^2/2 = 1 - V/V_0$.

супер, осталось подставить.

в итоге:

$$\boxed{I \propto N(V) = 2\pi n_0 \left[\frac{\vartheta_0^2}{4} - \left(\frac{1 - V/V_0}{\vartheta_0} - \frac{\partial_0}{2}\right)^2\right]} \tag{23.1}$$

В итоге видим, что корень квадратный фототока линейно зависит от запирающего напряжения.

Сделаем пару ключевых выводов:

мы можем с помощью 23.1 можем определить величину запирающего потенциала V_0, если измерим зависимость $\sqrt{I}(V)$

при изменении ω, зависимость V должна быть такой: $V_0(\omega) = (\hbar\omega - W)/e$.

Поэтому, строя график $V(\omega)$, мы ожидаем видеть прямую, по коэффициенту наклона которой можно определить постоянную Планка: $\frac{dV_0}{d\omega} = \frac{\hbar}{e}$.

Интересно, что такая зависимость будет одинаковой для любого вещества.

С помощью 23.1 мы можем можем определить величину запирающего потенциала, если измерим зависимость $\sqrt{I}(V)$

Виды фотоэффектов

из лабника спишу потом, пока не актуально.

О влиянии структуры твердых тел на фотоэффект (?????)

общефиз и опытные факты

(??? вообще мы его смотрим ведь только в твердых телах, а не в атомах в пространстве, чего тогде это будто бы не учитываем???)

Облучение проводящего шара и вылет конечного числа электронов

тупая задача для маги

Дано шар, столько-то электронов улетело, еще что-то..

На шаре образовывается положительный заряд, за счет которого однажды электронам не хватит энергии улететь на бесконечность.

Потенциальная энергия это

$$W_0 = q\varphi = q\frac{Q}{r}$$

где Q - заряд шара.

(кстати, она отрицательна, потому что q отрицательный, подумаю про это потом)

Величина барьера равна энергии выхода.

$$W_0 = T_e$$

В итоге формула фотоэффекта дает ответ

Формула Эйнштейна для фотоэффекта

Фотоэффект Нерелятивистский случай по Ландау 4

(подробнее в другой записи будет, тут суть напишу. сперва скорее всего просто выгрузки будут.)

Упрощенные формулы и суть (?)

Теория

В 49-52 мы рассматривали радиационные переходы (испускание или поглощение фотона) между атомными уровнями дискретного спектра. Фотоэффект отличается от такого процесса поглощения фотона лишь тем, что конечнсе состояние относится к непрерывному спектру.

Сечение фотоэффекта может быть вычислено до конца в аналитическом виде для атома водорода или для водородоподобного иона (с зарядом ядра $Z \ll 137$).

В начальном состоянии имеем электрон на дискретном уровне $\varepsilon_i \equiv -I$ (I- потенциал ионизации атома) и фотон с определенным нмпульсом k. В конечном состоянии электрон имеет импульс p (и энергию $\varepsilon_f \equiv \varepsilon$). Поскольку p пробегает непрерывный ряд значений, сечение фотоэффекта дается формулой

$$d\sigma = 2\pi \left|V_{fl}\right|^2 \delta(-I + \omega - \varepsilon)\frac{d^3p}{(2\pi)^3}$$

(ср. $(44, 3)$), причем волновая функция конечного состояния электрона предполагается нормированной на одну частицу в объеме $V = 1$. Таким же образом по-прежнему

нормирована волновая функция фотона; для. перехода к сечению do вероятность dw должна быть при этом разделена на плотность потока фотонов (равную $c/V = c$), но в релятивистских единицах это не отражается на виде формулы $(56, 1)$.

Выберем, как и в $(45, 2)$, трехмерно поперечную калибровку фотона. Тогда

$$V_{fi} = -e\mathbf{A}\mathbf{j}_{fi} = -e\sqrt{4\pi}\frac{1}{\sqrt{2\omega}}M_{fl}$$

где обозначено

$$M_{fi} = \int \psi'^{*}(\alpha \mathrm{e})e^{i\mathrm{kr}}\psi d^3x$$

($\psi \equiv \psi_i$ и $\psi' \equiv \psi_f$ - начальная и конечная волновые функции электрона). Заменив в $(56, 1) d^3p \to \mathbf{p}^2 d|\mathbf{p}|do = \varepsilon|\mathbf{p}|d\varepsilon do$ и проинтегрировав δ-функцию по $d\varepsilon$, перепишем эту формулу в-виде

$$d\sigma = e^2\frac{\varepsilon|\mathrm{p}|}{2\pi\omega}\left|M_{fi}\right|^2 do$$

Мы произведем вычисления в двух случаях, различающихся значением энергии фотона: для $\omega \gg I$ и для $\omega \ll m$. Поскольку $I \sim me^4Z^2 \ll m$, эти две области частично перекрываются (при $I \ll \omega \ll m$), так что исследование этих случаев дает по существу полное описание фотоэффекта. Начнем со случая

$$\omega \ll m$$

При этом скорость электрона мала как в начальном, так и в конечном состоянии, так что по отношению к электрону задача - целиком нерелятивистская. Соответственно этому заменим в $(56, 2)\boldsymbol{\alpha}$ нерелятивистским оператором скорости $\hat{\mathbf{v}} = -i\nabla/m$ (ср. 45). Кроме того, можно перейти к дипольному приближению - положить $e^{i\mathrm{kr}} \approx 1$, т. е. пренебречь импульсом фотона по сравнению с импульсом электрона. Тогда

$$d\sigma = e^2\frac{m|\mathbf{p}|}{2\pi\omega}\left|\mathbf{e}\mathbf{v}_{fl}\right|^2 do, \quad \mathbf{v}_{fi} = -\frac{i}{m}\int \psi'^{*}\nabla\psi \cdot d^3x. \qquad (56{,}5)$$

Будем рассматривать фотоэффект с основного уровня атома водорода (или водородоподобного иона). Тогда

$$\psi = \frac{(Ze^2m)^{3/2}}{\sqrt{\pi}}e^{-Ze^2mr}$$

(в обычных единицах $me^2 \to 1/a_0$, где $a_0 = \hbar^2/me^2$ - боровский радиус).

В качестве же ψ' надо взять волновую функцию, асимптос ней сходящуюся сферическую (см. III, 136, где такая функция обозначалась $\psi_{\mathrm{p}}^{(-)}$). В силу правила отбора по l переход из s-состояния возможен лишь в p-состояние (дипольный случай). Поэтому в разложении [1])

$$\psi_{\mathrm{p}}^{(-)} = \frac{1}{2p}\sum_{l=0}^{\infty} i^l(2l+1)e^{-i\delta_l}R_{pl}(r)P_l\left(\mathrm{nn}_1\right)$$

($\mathrm{n} = \mathrm{p}/p, \mathrm{n}_1 = \mathrm{r}/r$) достаточно оставить лишь член с$l = 1$, Опустив несущественные фазовые множители, получим

$$\psi' = \frac{3}{2p}\left(\mathrm{nn}_1\right)R_{p1}(r)$$

С функциями ψ и ψ' из (56, 6), (56, 8) имеем

$$\mathrm{ev}_{fi} = \frac{3\left(Ze^2m\right)^{5/2}}{2\sqrt{\pi}mp} \iint (\mathbf{nn}_1)\,(\mathrm{n}_1\mathrm{e})\, e^{-Ze^2mr} R_{p1}(r) do_1 \cdot r^2 dr =$$
$$= \frac{\sqrt{2\pi}\left(Ze^2m\right)^{5/2}}{pm}(\mathrm{ne}) \int\limits_0^\infty r^2 e^{-Ze^2mr} R_{p1}(r) dr.$$

Согласно III (36, 18) и III (36, 24) радиальная функция (в прннятых здесь единицах)

$$R_{p1} = \frac{\sqrt{8\pi}Ze^2m}{3}\sqrt{\frac{1+v^2}{v\left(1-e^{-2\pi v}\right)}}\ \mathrm{pre}\ e^{-ipr}F(2+iv, 4, 2ipr),$$

где обозначено:

$$v = \frac{Ze^2m}{p}\left(= \frac{Ze^2}{\hbar v}\right).$$

Нужный нам интеграл вычисляется с помощью формулы

$$\int\limits_0^\infty e^{-\lambda z} z^{\gamma-1} F(\alpha, \gamma, kz) dz = \Gamma(\gamma)\lambda^{\alpha-\gamma}(\lambda - k)^{-\alpha}$$

(см. III (f, 3)). Заметив также, что

$$\left(\frac{v+i}{v-i}\right)^{iv} = e^{-2v\,\mathrm{arcctg}\,v}$$

получим

$$\mathrm{ev}_{fi} = \frac{2^{7/2}\pi v^3(\mathrm{ne})}{\sqrt{p}m\left(1+v^2\right)^{3/2}} \frac{e^{-2v\,\mathrm{arcctg}\,v}}{\sqrt{1-e^{-2\pi v}}}$$

нергия ионизации с основного уровня атома водорода (или водородоподобного иона) $I = Z^2e^4m/2$. Поэтому

$$\omega = \frac{p^2}{2m} + I = \frac{p^2}{2m}\left(1+v^2\right)$$

Учитывая это соотношение, пишем окончательное выражение для сечения фотоэффекта с испусканием электрона в элемент телесного угла do:

$$d\sigma = 2^7\pi\alpha a^2 \left(\frac{I}{\hbar\omega}\right)^4 \frac{e^{-4v\,\mathrm{arcctg}\,v}}{1-e^{-2\pi v}}(\ \mathrm{ne}\ )^2 do,$$

где $a = \hbar^2/mZe^2 = a_0/Z$ (здесь и ниже - обычные единицы). Отметим, что угловое распределение фотоэлектронов определяется множителем $(\mathrm{ne}\ )^2$. Он максимален в направлениях, параллельных направлению поляризации падающих фотонов, и обращается в нуль в перпендикулярных вектору e направлениях, в том числе в направлении падения. Для неполяризованных фотонов формула (56, 11) должна быть усреднена по направлениям e, что сводится к замене

$$(\mathrm{ne})^2 \to \frac{1}{2}\left[\mathrm{n}_0\mathrm{n}\right]^2$$

где $\mathrm{n}_0 = \mathbf{k}/k$ (см. (45, 46)). Интегрирование же формулы (56,11) по углам дает полное сечение фотоэффекта:

$$\sigma = \frac{2^9\pi^2}{3}\alpha a^2 \left(\frac{1}{\hbar\omega}\right)^4 \frac{e^{-4v\,\mathrm{arcctg}\,v}}{1-e^{-2\pi\nu}}$$

(M. Stobbe, 1930). Предельное значение σ при $\hbar\omega \to I$ (т. е. $v \to \infty$):

$$\sigma = \frac{2^9\pi^2}{3e^4}\alpha a^2 = \frac{2^9\pi^2}{3e^4}\frac{\alpha a_0^2}{Z^2} = 0,23\frac{a_0^2}{Z^2}$$

(в знаменателе $e = 2,71...$).. Как и должно быть для реакции с образованием заряженных частиц (см. III, \$147), сечение фотоэффекта вблизи его порога стремится к постоянному пределі.

Случай же $\hbar\omega \gg I$ (причем по-прежнему $\hbar\omega \ll mc^2$) отвечает борновскому приближению ($v = Ze^2/\hbar v \ll 1$). Формула (56, 12), принимает вид

$$\sigma = \frac{2^8\pi}{3}\alpha a_0^2 Z^5 \left(\frac{I_0}{\hbar\omega}\right)^{7/2}$$

($I_0 = e^4m/2\hbar^2-$ энергия ионизации атома водорода). Процессом, обратным фотоэффекту, является радиационная рекомбинация электрона с неподвижным ионом. Сечение этого процесса ($\sigma_{\text{рек}}$) можно найти по сечению фотоэффекта (σ_ϕ) с помощью принципа детального равновесия (III, 144). Согласно этому принципу сечения процессов $i \to f$ и $f \to i$ (с двумя частицами в каждом из состояний i и f) связаны соотношением

$$g_l p_i^2 \sigma_{l\to f} = g_f p_f^2 \sigma_{f\to i}$$

где p_i, p_f - импульсы относительного движения частиц, а g_i, g_f - спиновые статистические веса состояний i и f. Учитывая также, что для фотона $g = 2$ (два направления поляризации), а статистический вес свободного электрона и иона равен статистическому весу основного состояния атома водорода, получаем для этого состояния

$$\sigma_{\text{рек}} = \sigma_\phi \frac{2\text{k}^2}{\text{p}^2}$$

)$\mathbf{p} = m\mathbf{v}$ - импульс падающего электрона, $\mathbf{k}$ - импульс испускаемого фотона). 3 а дачи 1. Получить формулу (56, 14) путем прямого использования борновского приближения в нерелятивистском случае.

Р е ше н и е. В борновском приближенни в качестве ψ' в формуле (56, 5) надо писать просто плоскую волну $\psi' = e^{i\text{pr}}$, а ψ - по-прежнему функция (56, 6). Тогда

$$\mathbf{v}_{ft} = \mathbf{v}_{if} = \frac{1}{m}\int \psi\hat{\mathbf{p}}\psi' d^3x = \frac{\mathbf{p}}{m}\frac{(Ze^2m)^{3/2}}{\sqrt{\pi}}\left(e^{-Ze^2mr}\right)_{\mathbf{p}'}$$

Фурье-компонента дается формулой (57, 66), так что

$$\mathbf{v}_{ft} \approx 8\sqrt{\pi}p^{-3}m^{3/2}\left(Ze^2\right)^{5/2}\mathbf{n}.$$

Подставив в (56, 5) и проинтегрировав по do, получим (56,14) (при этом, с достаточной точностью, $p^2/2m \approx \omega$). 2. Определить полное сечение радиационной рекомбннацни быстрого нерелятивистского электрона ($I \ll mv^2 \ll mc^2$) с ядром (заряд $Z \ll 137$).

р е ше н ие. Сечение захвата на K-оболочку (главное квантовое число $n = 1$) получается подстановкой (56, 14) в (56, 15) :

$$\sigma_1^{\text{рек}} = \frac{2^7\pi}{3}Z^5\alpha^3 a_0^2\left(\frac{I_0}{\varepsilon}\right)^{5/2}$$

)$\varepsilon = mv^2/2$ - энергия падающего электрона; $\omega \approx \varepsilon$). Из других состояний образующегося атома существенны лншь s-состояния: прн вычнсления матричного элемента в борновском

приближенни существенны значения волновой функции связанного состояния при малых r (как это будет видно из вычислений в 57), а при $l > 0$ эти значения малы по сравнению со значениями функций с $l = 0$; при этом достаточно учитывать два первых члена разложения ψ по степеням r. Для состояний с $l = 0$ и пронзвольным n эти члены

$$\psi = \frac{1}{\sqrt{\pi} a^{3/2} n^{3/2}} \left(1 - \frac{r}{a}\right)$$

т. е. содержат n лишь в виде общего множителя $n^{-3/2}$ (написанное выражение получается разложением функции III $(36, 13)$). Поэтому полное сечение рекомбинадни

$$\sigma^{\text{рек}} = \sum_{n=1}^{\infty} \sigma_n^{\text{рек}} = \sigma_1^{\text{рек}} \sum_{n=1}^{\infty} \frac{1}{n^3} = \zeta(3) \sigma_1^{\text{рек}}$$

(значение ζ-функщии: $\zeta(3) = 1,202$).

Фотоэффект Релятивистский случай по Ландау 4

(подробнее в другой записи будет, тут суть напишу. сперва скорее всего просто выгрузки будут.)

Упрощенные формулы и суть (?)

Теория

Обратимся к случаю $\omega \gg I$. $(57, 1)$ При этом также $\varepsilon = \omega - I \gg I$, и потому влияние кулонова поля ядра на волновую функцию фотоэлектрона (ψ') может быть учтено с помощью теории возмущении. Пишем ψ' в виде

$$\psi' = \frac{1}{\sqrt{2\varepsilon}} \left(u' e^{i\text{pr}} + \psi^{(1)}\right)$$

Фотоэлектрон может быть релятивистским; поэтожу невозмущенная функция в $(57, 2)$ напнсана в виде релятивистской плоской волны $(23, 1)$.

Хотя в начальном состоянии электрон нерелятивистский, в его волновой функции ф тем не менее должна быть (по выясняю; щимся ниже причинам) учтена релятивистская поправка ($\sim Ze^2$). Такая функция дается формулой (см. задачу к 39).

$$\psi = \left(1 - \frac{i}{2m} \gamma^0 \gamma \nabla\right) \frac{u}{\sqrt{2m}} \psi_{\text{нр}}$$

где ψ - нерелятивистская функция связанного состояния $(56, 6)$, а и-бнспинорная амплитуда покоящегося электрона, нормнрованная принятым нами условием $\bar{u}u = 2m$.

Подставим функцин $(57, 2 - 3)$ в матричный элемент $(56, 2)$[1]):

$$M_{fi} = \frac{1}{2\sqrt{m\varepsilon}} \int \left\{ \bar{u}'(\text{ve}) \left[\left(1 - \frac{i}{2m} \gamma^0 \boldsymbol{\gamma} \nabla\right) u \psi_{\text{up}}\right] e^{-i(\mathbf{p}-\mathbf{k})\mathbf{r}} + \right.$$
$$\left. + \bar{\psi}^{(1)}(\text{ve}) e^{i\text{kr}} u \Psi \right\} d^3x. \quad (57, 4)$$

Имея в виду получить первый член разложения этой величины по Ze^2, мы можем во втором члене в фигурных скобках замезультате такой замены обратился бы (при $\mathbf{p} - \text{k} \neq 0$) в нуль (именно поэтому в ф необходимо учитывать также и первую релятивистскую

поправку, пропорциональную Ze^2; при $v \sim 1$ эта поправка дает вклад в сечение того же порядка, что и следующий член разложения $\Psi_{\rm n}$ по Ze^2).

В первом члене в $(57,4)$ производим интегрирование по частям, переводя действие оператора ∇ с фир на экспоненциальный множитель. В результате получим

$$M_{fi} = \frac{(Ze^2m)^{3/2}}{2(\pi m\varepsilon)^{1/2}} \left\{ \bar{u}'(\mathrm{ve}) \left[1 + \frac{1}{2m} v^0 v(\mathbf{p} - \mathrm{k}) \right] u \left(e^{-Ze^2mr} \right)_{\mathrm{p-k}} + \right.$$
$$\left. + \bar{\psi} - \overset{(1)}{}_{-k}(\mathrm{ve}) u \right\}, \quad (57,5)$$

где векторный индекс означает пространственную компоненту Фурье. С точностью до члена $\sim Ze^{22})$

$$\left(e^{-Ze^2mr} \right)_{\mathrm{p-k}} = \frac{8\pi Ze^2m}{(\mathbf{p} - \mathbf{k})^4}.$$

1) Функция $(57,3)$ была получена дла расстояний $r \sim 1/mZe^2$, на которых поправочный член в ней относительного порядка величнны Ze. Но для основного состояния (а также и для всех вообще s-состояний) формула $(57,3)$ пригодна для любых r, поскольку пронзводная от чисто экспоненциальной функиии $(56,6)$ (а с нею и поправочнй член в $(57,3)$) всегда пропорциональна Ze^2. Это обстоятельство позволяет воспользоваться формулой $(57,3)$ в рассматриваемой задаче, в которой существенны малые r. (При $v \sim 1$ существенны $r \sim 1/\ \mathrm{m}$.) 2) Взяв компоненту Фурье от обеих сторон равенства

$$\left(\Delta - \lambda^2 \right) \frac{e^{-\lambda r}}{r} = -4\pi\delta(r),$$

получим

$$\left(\frac{e^{-\lambda r}}{r} \right)_{\mathbf{q}} = \frac{4\pi}{\mathbf{q}^2 + \lambda^2}.$$

Дифференцирование этого выражения по параметру λ дает

$$\left(e^{-\lambda r} \right)_{\mathrm{q}} = \frac{8\pi\lambda}{\left(q^2 + \lambda^2 \right)^2}$$

Для вычисления же компоненты Фурье $\psi^{(1)}_{\mathrm{k}}$ пишем уравнение, которому удовлетворяет функция $\psi^{(1)}$:

$$\left(\gamma^0\varepsilon + i\gamma\nabla - m \right) \psi^{(1)} = e \left(\gamma^\mu A_\mu \right) u' e^{i\mathrm{pr}} = -\frac{Ze^2}{r} \gamma^0 u' e^{i\mathrm{pr}}$$

(оно получается подстановкой $(57,2)$ в $(32,1)$). Применив к обеим сторонам этого уравнения оператор $(\gamma^0\varepsilon + i\gamma\nabla + m)$, получим

$$\left(\Delta + \mathbf{p}^2 \right) \psi^{(1)} = -Ze^2 \left(\gamma^0\varepsilon + i\gamma\nabla + m \right) \left(\gamma^0 u' \right) \frac{1}{r} e^{i\mathrm{pr}}.$$

причем в членах с Δ и $\boldsymbol{\nabla}$ производим обычным образом интегрирование по частям:

$$\left(\mathbf{p}^2 - \mathbf{k}^2 \right) \psi^{(1)}_{\mathbf{k}} = -Ze^2 \left(\gamma^0\varepsilon - \gamma\mathbf{k} + m \right) \left(\gamma^0 u' \right) \left(\frac{1}{r} \right)_{\mathbf{k-p}} =$$
$$= -\ Ze^2 \left(2\varepsilon\gamma^0 - v(\mathbf{k} - \mathbf{p}) \right) \left(\gamma^0 u' \right) \frac{4\pi}{(\mathbf{k} - \mathbf{p})^2}.$$

В последней строке учтено, что амплитуда u' удовлетворяет уравнению

$$\left(\varepsilon\gamma^0 - \mathbf{p} - m \right) u' = 0, \text{ или } \quad \left(\varepsilon\gamma^0 + \mathbf{p}\gamma - m \right) \gamma^0 u' = 0.$$

Отсюда находим

$$\bar{\psi}^{(1)}_{-\mathrm{k}} = \psi^{(\mathrm{I})}_{\mathrm{k}}\gamma^0 = 4\pi Ze^2\bar{u}'\frac{2\varepsilon\gamma^0 + \gamma(\mathrm{k}-\mathrm{p})}{(\mathrm{k}^2-\mathrm{p}^2)\,(\mathrm{k}-\mathrm{p})^2}\gamma^0.$$

Подставив $(57,6-7)$ в матричный элемент $(57,5)$, представим его в виде

$$M_{fi} = \frac{4\pi^{1/2}\,(Ze^2m)^{5/2}}{(\ell m)^{1/2}(\mathbf{k}-\mathbf{p})^2}\bar{u}'Au$$

где

$$A = a(\mathrm{ve}) + (\mathrm{ve})\gamma^0(\boldsymbol{\gamma}\mathbf{b}) + (\gamma\mathbf{c})\gamma^0(\gamma\mathrm{e}),$$

$$a = \frac{1}{(\mathbf{k}-\mathbf{p})^2} + \frac{\varepsilon}{m}\frac{1}{\mathbf{k}^2-\mathbf{p}^2}, \quad \mathbf{b} = -\frac{\mathbf{k}-\mathrm{p}}{2m(\mathrm{k}-\mathbf{p})^2}, \quad \mathbf{c} = \frac{\mathbf{k}-\mathbf{p}}{2m\,(\mathbf{k}^2-\mathrm{p}^2)}.$$

Сечение

$$d\sigma = \frac{8e^2\,(Ze^2m)^5\,|\mathbf{p}|}{\omega(\mathbf{k}-\mathbf{p})^4m}\,(\bar{u}'Au)\left(\bar{u}\bar{A}u'\right)do,$$

где $\bar{A} = \gamma^0A^+\gamma^0$ (см. §65). Это выражение надо еще просуммировать по конечным и усреднить по начальным направлениям спина электрона. Эти действия производятся по описанным ниже, в 65, правилам с помощью поляризационных матриц плотности начального и конечного состояний:

$$\rho = \frac{m}{2}\left(\gamma^0+1\right), \quad \rho' = \frac{1}{2}\left(\gamma^0\varepsilon - v\mathbf{p} + m\right)$$

(в начальном состоянии $\mathrm{p}=0, \varepsilon = m$). Они приводят к выражению

$$d\sigma = \frac{16e^2\,(Ze^2m)^5\,\lfloor\mathbf{p}\,|}{m\omega(\mathbf{k}-\mathbf{p})^4}\mathrm{Sp}\left(\rho'A\rho\bar{A}\right)do$$

Вычисление следа (с использованием формул (22,22)) представляет собой чисто алгебраическую операцию и приводит к следующему результату:

$$\mathrm{Sp}\left(\rho'A\rho\bar{A}\right) = \frac{m}{\varepsilon+m}[a\mathbf{p} - (\mathbf{b}-\mathbf{c})(\varepsilon+m)]^2 + \\ + 4m(\mathbf{be})[(\varepsilon+m)(\mathbf{ce}) + a(\mathrm{pe})]$$

(вектор e предполагается вещественным - линейная поляризация фотона).

Придадим формуле сечения фотоэффета окончательный вид, введя полярный угол θ и азимут φ направления p относительно направления $\mathbf{k}$ в качестве оси z и плоскости $\mathbf{k}$, e в качестве плоскости $xz($ так что $\mathrm{pe} = |p|\cos\varphi\sin\theta)$. При $\omega \gg I$ сохранение энергии можно записать в виде $\varepsilon - m = \omega$ (вместо $\varepsilon - m = \omega - I$). Легко проверить, что тогда

$$\mathbf{k}^2 - \mathbf{p}^2 = -2m(\varepsilon - m), \quad (\mathbf{k}-\mathbf{p})^2 = 2\varepsilon(\varepsilon-m)(1-v\cos\theta),$$

где $\mathbf{v} = \mathrm{p}/\varepsilon$ - скорость фотоэлектрона. После простых преобразований получим окончательно

$$d\sigma = Z^0\alpha^4r_e^2\frac{v^3\,(1-v^2)^3\sin^2\theta}{\left(1-\sqrt{1-v^2}\right)^5(1-v\cos\theta)^4}\times \\ \times\left\{\frac{\left(1-\sqrt{1-v^2}\right)^2}{2\,(1-v^2)^{3/y}}(1-v\cos\theta) + \right. \\ \left. + \left[2 - \frac{\left(1-\sqrt{1-v^2}\right)(1-v\cos\theta)}{1-v^2}\right]\cos^2\varphi\right\}do, \quad (57,8)$$

где $r_e = e^2/m$.

В ультрарелятивистском случае ($\varepsilon \gg m$) сечение фотоэффекта имеет резкий максимум при малых углах $\left(\theta \sim \sqrt{1-v^2}\right)$, т. е. электроны испускаются преимущественно в направлении падения фотона. Вблизи максимума пишем

$$1 - v\cos\theta \approx \frac{1}{2}\left[\left(1-v^2\right) + \theta^2\right]$$

и главные члены в $(57,8)$ дают

$$d\sigma \approx 4Z^5\alpha^4 r^2 \frac{\left(1-v^2\right)^{1/2}\theta^3}{\left(1-v^2+\theta^2\right)^3} d\theta d\varphi.$$

лементарное, хотя и довольно длинное интегрирование выражения $(57,8)$ по углам приводит.к следующей формуле для полного сечения (F. Sauter, 1931):

$$\sigma = 2\pi Z^5\alpha^4 r_e^2 \frac{\left(\gamma^2-1\right)^{2/}}{(\gamma-1)^5}\left\{\frac{4}{3}+\right.$$
$$\left.+\frac{\gamma(\gamma-2)}{\gamma+1}\left(1-\frac{1}{2\gamma\sqrt{\gamma^2-1}}\ln\frac{\gamma+\sqrt{\gamma^2-1}}{\gamma-\sqrt{\gamma^2-1}}\right)\right\}.$$

где для краткости введен «лоренцев множитель»

$$\gamma = \frac{1}{\sqrt{1-v^2}} = \frac{\varepsilon}{m} \approx \frac{m+\omega}{m}.$$

В ультрарелятивистском случае эта формула сводится к простому вьражению

$$\sigma = 2\pi Z^5\alpha^4 r_e^2/\gamma$$

В случае же $I \ll \omega \ll m$ переход в $(57,10)$ пределу малых $\boldsymbol{\gamma} - 1$ приводит к известному уже нам результату $(56,14)$.

Theory of photoeffect for XPS method

Об истории открытия фотоэффекта (?)

(тоже потом укажу.)

23.2.2 Young's Double-Slit Experiment

Обсудим подробно опыт Юнга.

Об опыте Юнга

(конкретно, в каких параметрах установки он будет?)

Один из самых важнейших опытов квантовой механики, дающий пояснение, что такое суперпозиция состояний - это опыт Юнга

оценки параметров для опыта Юнга (?)

тоже важно, но сперва это пропишу в оптике.

Важно понимать, какие параметры системы и почему они такие, чтобы была возможность воспроизводить опыт Юнга.

???

Связь с невозможностью этого опыта с отсутствией дырки в барьере до барьера с двумя щелями (!?!??!?)

(??? где мы учитываем, что он на самом деле обязателен??? вообще хз, казалось бы...)

Опыт Юнга и переход в классику по Фельдбругге (!!??!??!?!?!)

(про это остаются вопросы, тем не менее, теория крутая и полезная.)

Обсудим описание эксперимента Юнга как пример применения теории Пикара-Лефшеца.

мотивация

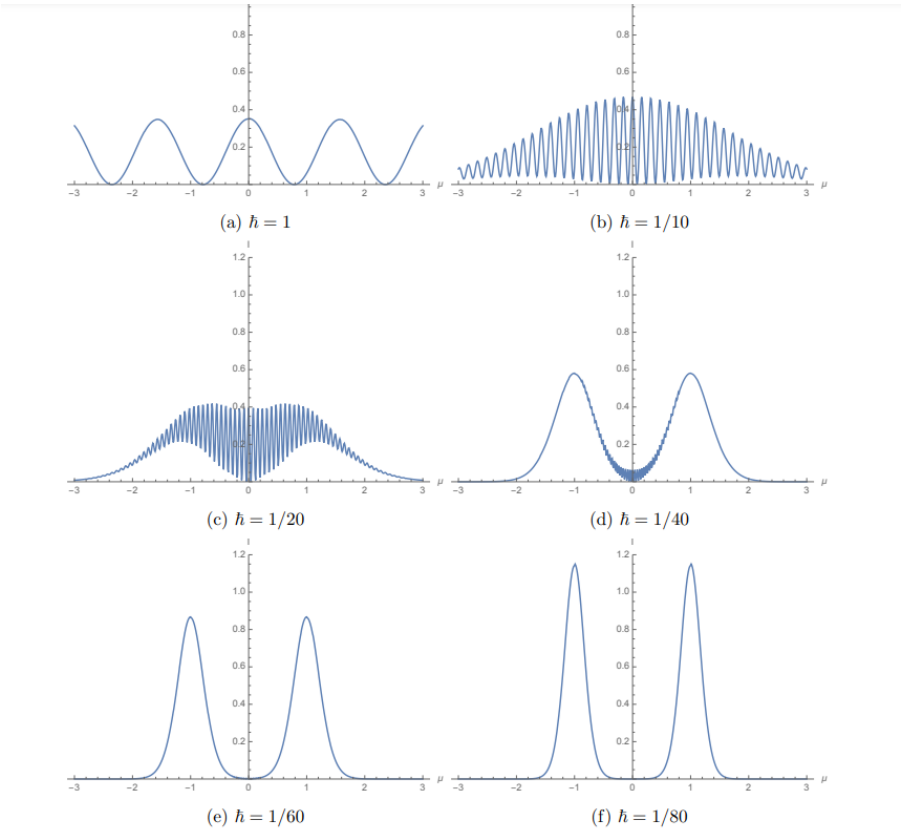
Опыт Юнга интересно изучить, потому что с одной стороны это один из самых популярных квантовых экспериментов, с другой - прекрасный способ применить методы, разработанные при изучении гравитационного линзирования.

Также вокруг него существует много домыслов и неверных трактовок, с которыми можно в корне неверно начать понимать квантовую механику, поэтому иметь четкое представление о нем крайне полезно.

Несмотря на чрезвычайную простоту этого примера и его центральную роль в идейном понимании квантовой физики и оптики, детальные интерференционные картины на удивление трудно вычислить.

модель опыта Юнга в двух словах

??? а там кстати не классическая это дифракция ведь, нет??
именно квантовые эффекты???
что там квантового?



(a) $\hbar = 1$ (b) $\hbar = 1/10$ (c) $\hbar = 1/20$ (d) $\hbar = 1/40$ (e) $\hbar = 1/60$ (f) $\hbar = 1/80$

Дифракционная картина опыта Юнга сполна находится возведением в квадрат $I(\mu) = |\Psi(\mu)|^2$ амплитуды $\Psi(\mu)$, которая имеет вид

$$\Psi(\mu) = \mathcal{N} \int e^{\frac{i}{\hbar}(x-\mu)^2} T(x) dx,$$

где $\mathcal{N}$ - нормировочный множитель, а $T(x)$ - функция пропускания:

$$T(x) \propto \exp\left[\frac{\epsilon}{\epsilon^2 + (x-s_1)^2} + \frac{\epsilon}{\epsilon^2 + (x-s_2)^2} - \frac{1}{\epsilon}\right]$$

описание опыта Юнга

(темы статьи Турока)

Изучим дифракционную картину от пары гладких щелей конечного размера.

Посмотрим, как меняется дифракционная картина в классическом пределе, то есть когда $\hbar$ приравнивается к нулю.

Требуется обобщение, чтобы сделать интерференционную "фазу" комплексной, чтобы заглушить амплитуду вдали от двух узких щелей.

Моделируя эту сложную фазу с помощью простой рациональной функции, легко находятся наперстки Лефшеца и вычисляется интерференционная картина при всех значениях параметров.

функция пропускания

Рассмотрим удаленный точечный источник, излучающий частицы в направлении экрана, с тонким барьером, отделяющим экран от источника.

Барьер за исключением двух щелей, непрозрачен для частиц.

??? я не знаю, как другие делают люди решение этой задачи, но тут я так понял, суть метода в том, что такой вид функции пропускания с одной стороны физически абсолютно верный, с другой - аналитически хорошо продолжается, именно поэтому мы такой выбрали.

В безразмерных координатах, которые будут определены ниже, ???????амплитуда проходящего света имеет вид

$$T(x) \propto \exp\left[\frac{\epsilon}{\epsilon^2 + (x-s_1)^2} + \frac{\epsilon}{\epsilon^2 + (x-s_2)^2} - \frac{1}{\epsilon}\right]$$

состоящий из двух пиков, каждый интенсивностью равным единицей с центром в $x = s_1$ и $x = s_2$ соответственно.

Здесь, $\epsilon > 0$ это небольшое число, отражающее небольшую ширину щелей в непрозрачном барьере.

(место вставить рисунок-иллюстрацию)

Вдали от щелей имеем зависимость $T \sim \exp(-1/\epsilon)$.

амплитуда прохождения

!!! тут используется в точности теория из оптики, которую нужно сперва прописать, потом будут понятны формулы.

Предполагая, что амплитуда падающих частиц когерентна и постоянна через щели, мы можем затем вычислить интегральную амплитуду пути как и делали ранее.

Однако здесь мы имеем дело с частицей фиксированной массы m, энергии E и импульса $p = \sqrt{2mE}$.

Последняя формула в $S_r[\boldsymbol{x}] = \int_{x_i}^{x_f} |d\boldsymbol{x}||\boldsymbol{p}|$, в тех же малых приближениях смещения, сделанных в уравнении $\Psi\left(\boldsymbol{x}_{\text{obs}}, \boldsymbol{x}_s; \nu\right) \propto \int d\boldsymbol{x} \exp\left[i\frac{\omega}{2c}\left(\frac{(\boldsymbol{x}-\boldsymbol{\mu})^2}{d} - \frac{\Sigma_e(\boldsymbol{x})e^2}{m_e\epsilon_0\omega^2}\right)\right]$, выше, ??????? дает пифагорейский вклад в фазу, $p(x-\mu)^2/(2d\hbar)$, где d-расстояние от щелей до экрана.

Установив $x \to xa$, где a - характерный размер щелей, а x - безразмерный, мы примем величину $\hbar 2d/\left(pa^2\right)$ за нашу новую, безразмерную $\hbar$.

В терминах этих безразмерных величин амплитуда для частицы, чтобы прибыть в положение μ на экране, следовательно, задается осциллирующим интегралом

$$\Psi(\mu) = \mathcal{N} \int e^{\frac{i}{\hbar}(x-\mu)^2} T(x) dx$$

с константой нормализации $\mathcal{N}$, обеспечивающей унитарность $\int |\Psi(\mu)|^2 \, d\mu = 1$.

Вероятность того, что частица достигнет μ на экране, задается абсолютным квадратом волновой функции

$$I(\mu) = |\Psi(\mu)|^2$$

Заметим, что безразмерная версия постоянной Планка $\hbar$ появляется в этой нерелятивистской задаче, тогда как она отменяется из наших более ранних формул для безмассовой частицы в результате масштабной ковариации последней. (????)

Вычислим волновую функцию за счет аналитического продолжения экспоненты

$$\phi(x;\mu) = \frac{i}{\hbar}(x-\mu)^2 + \frac{\epsilon}{\epsilon^2 + (x-s_1)^2} + \frac{\epsilon}{\epsilon^2 + (x-s_2)^2} - \frac{1}{\epsilon},$$

и вычисления наперстка Лефшеца.

(???) Экспонента имеет 4 полюса и 9 седловых точек.

Полюсы в точке $x = s_i \pm i\epsilon$ соответствуют щели с центром в точке s_i. Седловые точки являются корнями многочлена девятого порядка.

Мы можем связать четыре седловые точки с каждой щелью.

Оставшаяся седловая точка является общей и перемещается между полюсами, соответствующими двум щелям, в зависимости от положения на экране μ.

тут на рис. показаны соответствующие диаграммы Пикара-Лефшеца для различных положений μ для $\hbar = 1$.

В описании мы для простоты предположим, что левая щель находится в точке s_1, а правая-в точке s_1.

щель должна быть на уровне s_2, то есть $s_1 < s_2$:

анализ диаграмм Пикара-Лефшеца для эксперимента Юнга

- Для позиций на экране далеко слева от щелей, $\mu \ll_1$, наперсток состоит из пяти самых крутых контуров спуска.

Наперсток проходит от нижнего левого угла к верхнему правому через сложную седловую точку.

Затем наперсток обвивается вокруг верхнего левого и верхнего правого полюсов.

Для позиций $\mu \leq \frac{s_1+s_2}{2}$ в волновой функции доминирует левая щель.

Поэтому неудивительно, что наперсток, соответствующий правой щели, является репрезентативным в этом режиме.

- Когда μ приближается к s_1, мы наблюдаем преобразования Стокса, после которого релевантны только четыре седловые точки.

Наперсток перемещается из нижнего левого угла через седловую точку в верхний левый полюс, после чего он проходит через седловую точку между двумя левыми полюсами.

Правая часть наперстка практически не изменилась.

- Когда μ приближается к средней точке $\frac{\mu_1+\mu_2}{2}$, мы наблюдаем, что комплексная седловая точка становится актуальной (?) после явления Стокса.

Наперсток теперь состоит из четырех контуров наискорейшего спуска.

- Для μ вблизи средней точки $\mu = \frac{\mu_1+\mu_2}{2}$ мы наблюдаем, что после еще одного стоксова перехода мы получаем наперсток, состоящий из пяти самых крутых контуров спуска.

Обратите внимание, что средняя седловая точка переместилась в начало координат $x = 0$.

Когда положение μ будет еще больше увеличено, эта седловая точка переместится к полюсам, соответствующим правой щели. Соответствующие диаграммы Пикара-Лефшеца являются зеркальными отражениями рассмотренных выше.

(тут снова можно вставлять крышесносные диаграммы Пикара-Лефшеца)

В квазиклассическом пределе $\hbar \to 0$ геометрия наперстка Лефшеца во все большей степени определяется пифагорейским членом в уравнении (B4).

Как следствие, после нескольких преобразований Стокса восемь седловых точек, которые могут быть связаны с полюсами, соответствующим двум щелям, становятся более тесно связанными с полюсами, представляющими геометрию правой части наперстка на рис.37.

Оставшаяся седловая точка все еще движется между полюсами, соответствующими двум щелям.

Однако заметим, что в интеграле все больше доминируют две седловые точки между четырьмя полюсами.

Эти две седловые точки приближаются к реальной линии при $x = s_1$ и $x = s_2$ в этом пределе.

Учитывая наперсток, мы можем эффективно оценить осциллирующий интеграл для различных $\hbar$

(см. рис. 38).

Для относительно больших $\hbar$ интенсивность на экране доминирует из-за интерференционных эффектов.

Как для $\hbar = 1$, так и для $\hbar = 1/2$ мы не наблюдаем классических пиков интенсивности, соответствующих двум щелям.

В квазиклассическом пределе, $\hbar \to 0$, интерференционная картина медленно заменяется классическими пиками.

(вот это явно покажу!!!)

Заметим, что этот переход от квантового к классическому режиму не может быть исследован в традиционном тонкощелевом приближении.

Заметим, что в то время как в поведении сильных линз преобладают каустики, где седловые точки вырождаются, качественное поведение двухщелевого эксперимента полностью определяется стоксовыми преобразованиями.

Седловые точки всюду невырождены, и h - функция является функцией Морса.

В обоих случаях аппроксимация седловой точки не работает, и интеграл должен оцениваться вдоль всего наперстка Лефшеца.

Мы ожидаем, что это будет общей чертой квантовомеханических интерференционных явлений.

вид диаграмм

Приведем интерференционные диаграммы.
(когда дойду - почитаю эи интегралы, приведу картинки. вряд ли скоро дойду)

Типичное квантовое описание

для сравнения приведем также типичное описание этого эксперимента, которое многим известно.
(я не помню пока, из оптики допишу)

программный расчет

Приведем строчки кода, которые можно вставить в итоговый файл и посчитать диаграммы.
Функция, введенная в Wolfram, соответствующая опыту Юнга, имеет вид:

```
[Alpha] = 1;
f[x_, μ_]:= I ((x - μ)^2 + [Alpha]/([Alpha]^2 + (x + 0.5)^2) + [Alpha]/([Alpha]^2 + (x -
    0.7)^2) + 1/[Alpha]);
```

Где учтено, что если свет падает сразу на 2 щели, без вначале 1-й, то эффекта не будет? (??)

(??? не понимаю это пока что. мб оптика поможет понять.)

О заблуждениях про опыт Юнга

23.2.3 Experiment on the Compton Effect

Обсудим вмеру подробно эффект Комптона.
(maybe I'll move theory about it to some parts before)

Суть эффекта Комптона

(a paragraph with main ideas from theory about it)
Суть в том, что если фотон рассеивается на электроне, то длина волны фотона изменяется и она зависит от угла, на который он рассеивается. Соотношение следующее

$$\lambda - \lambda_0 = \frac{h}{mc}(1 - \cos\theta)$$

Для работы с ней, часто нужно подставлять длину волны через энергию $\lambda = hc/E$
(тут мб вывод в пару строк соберу, вроде обычные законы нужно использовать)

Определение 23.1. *Эффект Комптона - увеличение длины волны рассеянного излучения в сравнении в падающим.*

$$\begin{gathered} mc^2 + \hbar\omega_0 = \gamma mc^2 + \hbar\omega_1 \\ \frac{\hbar\omega_0}{c} = \gamma mv\cos\varphi + \frac{\hbar\omega_1}{c}\cos\theta \\ \gamma mv\sin\varphi = \frac{\hbar\omega_1}{c}\sin\theta \end{gathered}$$

Solution:

$$\Delta\lambda = \lambda_1 - \lambda_0 = \frac{h}{mc}(1 - \cos\theta) = \lambda_K(1 - \cos\theta)$$

λ_1 is the wavelength after scattering, $\lambda_K = \frac{h}{mc} = 2,42 \cdot 10^{-10}$cm - Compton wavelength.

In practice it is more conventional to measure the energies, not the wavelengths, of the scattered photons.

For a given incident energy, the outgoing final-state photon energy $E_\gamma = hc/\lambda$, $E_{\gamma'}$, is given by

$$E_{\gamma'} = \frac{E_\gamma}{1 + (E_\gamma/m_e c^2)\,(1 - \cos\theta)}$$

the same:

$$\nu' = \nu \frac{1}{1 + \frac{h\nu}{m_e c^2}(1 - \cos\theta)}$$

KleinNishina formula cross sections

The *KleinNishina* formula:

$$\sigma_k = 2\pi r_0^2 \left(\frac{1+\epsilon}{\epsilon^2} \left(\frac{2+2\epsilon}{1+2\epsilon} - \frac{\ln(1+2\epsilon)}{\epsilon} \right) + \frac{\ln(1+2\epsilon)}{2\epsilon} - \frac{1+3\epsilon}{(1+2\epsilon)^2} \right)$$

in another words,

$$\frac{d\sigma}{d\Omega} = \frac{1}{2} r_e^2 \left(\frac{\lambda}{\lambda'} \right)^2 \left[\frac{\lambda}{\lambda'} + \frac{\lambda'}{\lambda} - \sin^2(\theta) \right]$$

where $r_c = \hbar/m_e c$, α is the fine structure constant.
$r_e = \alpha r_c$
if $\hbar\omega \gg m_0 c^2$

$$\sigma_k = \frac{\pi r_0^2}{\epsilon} \left(\frac{1}{2} + \ln(2\epsilon) \right) = \pi r_0^2 \frac{m_0 c^2}{\hbar\omega} \left(\ln \frac{2\hbar\omega}{m_0 c^2} + \frac{1}{2} \right)$$

Intensity:

$$I' = \frac{I}{R^2} \frac{\omega'}{\omega} \frac{d\sigma}{d\Omega}$$

Thompson's scattering

If we speak about connected electrons, for them incoming wave make electrons hesitate on the same frequency, and it is called *Thompson's scattering.*

There two different properties of scattering cross section in this two effects.

комптоновская длина волны

она наверное слишком важная, поэтому оставлю себе напоминание, что нужно порешать задачи на ее применение.

Границы применимости эффекта Комптона для разных материалов

если у этого материала валентные электроны имеют энергию намного менее чем энергия гамма кванта.

и это же говорит о том, что можно считать электрон покоящимся

(потом лучше проработаю)

Экспериментальные свойства

общефиз и опытные факты

Обзор применений эффекта Комптона

Минимальная энергия гамма кванта от аннигиляции э-поз пары после рассеяния на графитовой мишени

Определить минимальную энергию гама-кванта образовавшегося в результате аннигиляции электрон-позитронной пары при его рассеянии на валентных электронах графитовой мишени. Дать численный ответ в электрон-вольтах. Энергия покоя для электрона $E_0 = 0,51$ МэВ.

Просто знаем, что родятся 2 гамма кванта, и просто у каждого будет такая же энергия, как и у электрона. А минимальная энергия - при максимальной длине волны, а по формуле Комптона это происходит при $\cos = -1$, то есть при рассеянии назад. Подставляя длину волны $\lambda = hc/E$

(короче тут тривиально всё считается)

тупо в итоге энергия в 3 раза меньше.

23.2.4 Davisson–Germer Experiment (?)

Опыт Дэвиссона-Джермера - физический эксперимент по дифракции электронов, проведённый в 1927 г.

американскими учёными Клинтоном Дэвиссоном и Лестером Джермером.

В нем наблюдалась дифракция электронов на кристаллической решётке монокристалла.

говорят, что это с УШ связано, а также с волнами де бройля, да я хз.

23.2.5 Franck–Hertz Experiment (??)

(?? важно суть его описать!!)

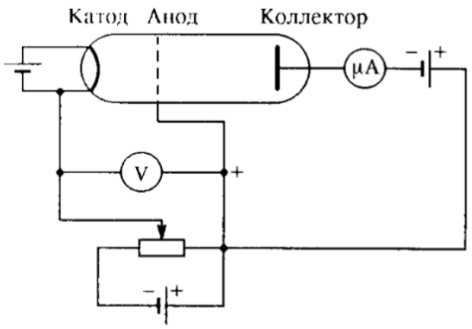
Это классический эксперимент, доказывающий, что у атомов дискретный уровень энергии.

Между катодом и анодом помещается гелий, далее увеличивая напряжение будем мерить проходящий ток.

В итоге зависимость показана на рисунке **??**

Об экспериментальной установке

Сперва остановимся на экспериментальной установке



23.2.6 Thomson Experiment

(редко его упоминают)

мотивация

Обсудим, для чего и насколько важно понимать опыт Юнга.
??? Опыт Юнга важен как мысленный эксперимент для понимания суперпозиции.
Для всего остального он бесполезен, так что копать тут нечего.

описание эксперимента

подробно, при каких условиях что получается?

объяснение

самое важное.
пока хз.
????

электрон не проходит через две щели одновременно

Согласно копенгагенской интерпретации, у нас электрон всегда локализован как частица.

заморочки про электрон и дырки (???)

зависимость от величины $\hbar$

тоже такая есть, я не шарю.

обзор неверных пониманий

Опыт Юнга интересен тем, что можно про него совершенно неправильно думать, так уйти в тупик по физике и на этом закончится всё обучение.
так что очень важно не затупить в нем.

23.2.7 Lasers

Обсудим минимальное, что хорошо бы знать о лазерах.
(пока в других разделах про это не предполагается теория.)

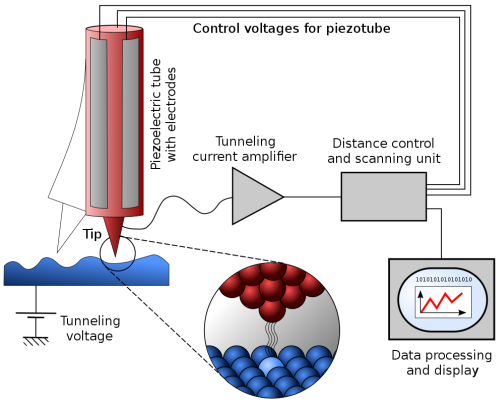
Принцип работы лазера

23.2.8 Microscopes

(currently, the idea is to write its main concepts)

On Scanning tunneling microscope

(см вики, страница где-то будет про него у меня тут для полноты, подробнее - в отдельной записи, мб в записи про наночастицы.)



24 Advanced Established Theoretical Methods of Quantum Mechanics

24.1 More About the Path Integral

Об источнике и производящем функционале по Киселеву

(только коротко укажу, что там есть. пишу под конец записи, потому что это максимально не приоритетная тема!!!)

Об интеграле по траекториям для инстантонов (!???)

(пока такой мелкий раздел, потому что где-то в другом месте по идее должна быть эта теория.)

Постановка задачи

На данном семинаре мы будем искать туннельное расщепление в двухъямном потенциале, следуя классической обзорной работе [Вай +82. Для удобства мы положим массу частицы $m = 1$, а потенциал зададим в виде $U(x) = \lambda\left(x^2 - \eta^2\right)^2$, и тем самым Гамильтониан задачи имеет следующий вид:

$$\hat{H} = -\frac{1}{2}\partial_x^2 + \lambda\left(x^2 - \eta^2\right)^2$$

Потенциал имеет пару минимумов в точках $x = \pm\eta$, вблизи которых он имеет осцилляторное разложение $V(x) = \frac{1}{2}\omega^2 x^2$, с частотами $\omega^2 = 8\lambda\eta^2$. Высота барьера, разделяющего эти две ямы, равна $U(0) = \lambda\eta^4$; поэтому квазиклассическому приближению соответствует $\lambda\eta^6 \gg 1 \Leftrightarrow \omega\eta^2 \gg 1$. Именно в таком приближении мы и будем решать эту задачу. На самом деле, её мы уже обсуждали в семинаре, посвящённому квазиклассическому приближению; в частности, мы вычисляли расщепление n-того осцилляторного уровня (на симметричные и антисимметричные комбинации). Квазиклассическое приближение, впрочем, работает только при $n \gg 1$; а сейчас мы сфокусируемся на расщеплении основного состояния $n = 0$. Для вычисления, мы воспользуемся слегка модифицированным аппаратом функций Грина, и функциональным интегралом.

Виковский поворот и Евклидово действие

Удобнее всего исследовать свойства основного состояния в мнимом времени $t = -i\tau$[4]. Функцию Грина во мнимом времени мы будем обозначать следующим образом [5]:

$$G_E(x,y,\tau) \equiv G(x,y,-i\tau) = \left\langle x \left| e^{-\hat{H}\tau} \right| y \right\rangle = \sum_n \psi_n(x)\psi_n^*(y)e^{-E_n\tau}$$

Обратим внимание, что чем выше возбуждение, тем меньший вклад оно даёт в эту сумму. Поэтому, в принципе, если рассмотреть $\tau = \beta \to +\infty$, то главный вклад останется только от основного (и, в нашем случае - первого возбуждённого) состояния. Именно этот случай мы и будем исследовать.

Для Евклидовой функции Грина можно вывести представление через функциональный интеграл, полностью эквивалентно тому, что мы делали на предыдущем семинаре. Ответ, в действительности, будет таким же, как если бы мы попросту в действие сделали формальную подстановку $t = -i\tau$. При этом:

$$iS[x(t)] = i\int \left[\frac{1}{2}\left(\partial_t x\right)^2 - U(x(t))\right] dt = -\int \left[\frac{1}{2}\left(\partial_\tau x\right)^2 + U(x(\tau))\right] d\tau \equiv -S_E[x(\tau)]$$

$$G_E(x,y,\beta) = \int\limits_{x(-\beta/2)=y}^{x(\beta/2)=x} \mathcal{D}x(\tau) \exp\left(-\int\limits_{-\beta/2}^{\beta/2} d\tau \left[\frac{1}{2}\left(\partial_\tau x\right)^2 + U(x(\tau))\right]\right)$$

Последнее называют «Евклидовым действием», и, как мы видим, оно отличается от обычного только изменением знака у потенциала $U(x)$ - тем самым, с классической точки зрения оно описывает движение в перевёрнутом потенциале. В дальнейшем нижний индекс «E» мы будем опускать, помня, что мы отныне работаем в мнимом времени.

Метод перевала

Поскольку $U(x)$ представляет собой полином четвёртой степени, мы имеем дело с нелинейным действием и с негауссовым функциональным интегралом. Брать этот интеграл мы будем методом перевала, который соответствует нахождению классических траекторий, минимизирующих действие - и квадратичному разложению вблизи них. Две тривиальных классических траектории очевидны - они соответствуют покоящимся частицам в точках $x(t) = \pm\eta$. Действие на них равно нулю, а квадратичное разложение устроено так же, как и для квантового гармонического осциллятора; и они дадут соответствующий вклад в следующие функции Грина в совпадающих точках, связанной с посчитанной на предыдущем семинаре функцией Грина квантового гармонического осциллятора $G_0(\beta)$ (с массой $m = 1$):

$$G^{(0)}(\eta,\eta,\beta) = G^{(0)}(-\eta,-\eta,\beta) \simeq G_0(\beta) = \sqrt{\frac{\omega}{2\pi\sinh(\beta\omega)}} \approx \sqrt{\frac{\omega}{\pi}}e^{-\beta\omega/2}$$

Из этого мы действительно видим, что в ведущем приближении имеется (двукратно вырожденный) осцилляторный уровень энергии $E = \omega/2$; но это не то, что нас интересует - нас интересует туннельное расщепление! Туннелированию соответствует переход из левой ямы в правую, поэтому именно такую функцию Грина мы будем считать: $G_E(\eta,-\eta,\beta)$.

Логика

Давайте вспомним, как мы берём многомерные интегралы методом перевала $I = \int \exp(-f(\boldsymbol{x}))d^d\boldsymbol{x}$. Рецепт прост: мы сперва мы ищем максимум, решая седловое уравнение (или систему уравнений) $\frac{\partial f(\boldsymbol{x}_0)}{\partial x_i} = 0$ - и находя решение, точку $\boldsymbol{x}_0$. В ведущем приближении, значение интеграла даётся значением функции в этой точке: $I \approx \exp\left(-f\left(\boldsymbol{x}_0\right)\right)$. Затем мы рассматриваем квадратичное разложение вблизи седловой точки: $f\left(\boldsymbol{x}_0+\boldsymbol{z}\right) \approx f\left(\boldsymbol{x}_0\right) + \frac{1}{2}\frac{\partial^2 f}{\partial x_i \partial x_j} z_i z_j$; и, наконец, берём гауссов интеграл:

$$I \approx e^{-f(\boldsymbol{x}_0)} \int d^d\boldsymbol{z} \exp\left(-\frac{1}{2}L_{ij}z_i z_j\right) = \frac{1}{\sqrt{\det \frac{\hat{L}}{2\pi}}} e^{-f(\boldsymbol{x}_0)}$$

Функциональный интеграл в этом смысле ничем не отличается - и мы применим этот рецепт и тут.

Седло

11.4.5 Седло Итак, нам нужно найти классическую траекторию $x_{cl}(\tau)$, удовлетворяющую экстремуму действия с граничными условиями $x(-\beta/2) = -\eta$ и $x(\beta/2) = \eta$:

$$\frac{\delta S_E}{\delta x(\tau)} = 0 \Rightarrow \partial_\tau^2 x = U'(x(\tau))$$

Данное уравнение можно решить в квадратурах, но проще всего решение устроено, если тут сразу взять предел $\beta \to \infty$. В таком случае, траектории соответствует перекатывающаяся за бесконечное время частица из левого «горба» перевёрнутого потенциала на правый. Чтобы найти эту траекторию, можно воспользоваться законом сохранения «энергии» $E = \frac{1}{2}\left(\partial_\tau x\right)^2 - U(x(\tau)) = \text{const}$ (на нашей траектории $E = 0$), благодаря чему понизить степень уравнения до первой:

$$\frac{1}{2}\left(\partial_\tau x\right)^2 = U(x(\tau)) \Rightarrow \frac{dx}{\eta^2 - x^2} = \sqrt{2\lambda}d\tau \Rightarrow x_{cl}(\tau) = \eta \tanh\frac{\omega\tau}{2}$$

Такую траекторию - нетривиальный экстремум нелинейного действия в функциональном интеграле - называют инстантоном.

Тут мы сталкиваемся с важной особенностью задачи. Вместо одной седловой траектории, мы, в действительности, имеем дело с целым седловым многообразием $x_{cl}\left(\tau - \tau_c\right)$, параметризуемым вещественным числом τ_c - положением инстантона. Наличие этой свободны, конечно, связано с трансляционной инвариантностью по времени - мы ведь взяли предел $\beta \to \infty$! Инстантон имеет характерную ширину $\sim \omega^{-1}$, которая мала (в частности, $\omega^{-1} \ll \beta$), и поэтому краевые эффекты, связанные с удержанием конечного β, будут экспоненциально малы на фоне основного результата, и в ведущем порядке они действительно не важны. Величина же τ_c с этой же точностью может пробегать все значения $\tau_c \in (-\beta/2, \beta/2)$. К этой свободе выбора центра инстантона мы ещё вернёмся, а пока давайте рассмотрим одно седло на этом многообразии, скажем, $\tau_c = 0$.

Итак, в главном порядке значение интеграла определяется действием на этом инстантоне. Давайте его вычислим (для этого удобно воспользоваться «законом сохранения энергии» и выразить член с потенциальной энергией через кинетическую):

$$S_0 = \int\limits_{-\infty}^{\infty} d\tau \left(\partial_\tau x_{cl}\right)^2 = \frac{2}{3}\omega\eta^2 \gg 1$$

Несложно убедиться, что это действие тождественно совпадает с «квазиклассическим действием» $\int\limits_{-\eta}^{\eta} p(x)dx$, которое определяло бы расщепление в квазиклассическом приближении.

Квадратичное разложение

Следуя логике метода перевала, нам нужно провести квадратичное разложение вблизи инстантона:

$$S_E\left[x_{cl}(\tau)+z(\tau)\right] \approx S_0 + \frac{1}{2}\int\limits_{-\beta/2}^{\beta/2} d\tau \left[(\partial_\tau z)^2 + U''\left(x_{cl}(\tau)\right) z^2(\tau)\right] \equiv S_0 + S_2[z(\tau)]$$

В квадратичном разложении действия стоит линейный оператор $\hat{L} = -\partial_\tau^2 + U''\left(x_{cl}(\tau)\right)$, спектр которого нам предстоит исследовать при взятии гауссового интеграла по квадратичным флуктуациям. Ответ тем самым с точки зрения метода перевала устроен следующим образом:

$$G(\eta,-\eta,\beta) \approx e^{-S_0} \int\limits_{z(-\beta/2)=0}^{z(\beta/2)=0} \mathcal{D}[z(\tau)] e^{-S_2[z(\tau)]}$$

Явный вид оператора следующий:

$$U''\left(x_{cl}(\tau)\right) = \frac{\omega^2}{2}\left(3\tanh^2\frac{\omega\tau}{2} - 1\right) = \omega^2\left(1 - \frac{3/2}{\cosh^2\frac{\omega\tau}{2}}\right)$$

Спектр оператора

11.4.7 Спектр оператора Итак, для взятия гауссового интеграла по $z(\tau)$ нам необходимо исследовать свойства (спектр) оператора $-\partial_\tau^2 + U''\left(x_{cl}(\tau)\right)$. Задача на его собственные значения ϵ_n и собственные функции $\psi_n(\tau)$ выглядит следующим образом:

$$\left(-\partial_\tau^2 - \frac{3\omega^2/2}{\cosh^2\frac{\omega\tau}{2}}\right)\psi_n(\tau) = \left(\epsilon_n - \omega^2\right)\psi_n(\tau)$$

Данное уравнение выглядит в точности как уравнение Шрёдингера в потенциале $\frac{1}{\cosh^2 x}$, решение которого нам известно - оно выражается через гипергеометрическую функцию ${}_2F_1$, и мы его обсуждали на четвёртом семинаре прошлого семестра. Воспользуемся ответами из того семинара, в которые нужно подставить следующие значения параметров:

$$m = \frac{1}{2}, \quad a = \frac{2}{\omega}, \quad U_0 = \frac{3\omega^2}{2}$$

Важным для исследования потенциала оказываются следующие два безразмерных параметра:

$$u = \frac{U_0}{1/2ma^2} = 6, \quad s = \frac{1}{2}(\sqrt{1+4u}-1) = 2$$

Дискретный спектр Как мы помним, число s характеризует количество связанных состояний. Для энергий $E_n \equiv \epsilon_n - \omega^2$ работает следующая формула: (число $n = 0, 1, ...$ и

$n < s$). Кроме того, целые числа s соответствуют случаю возникновению в яме связанного состояния (что означает, что есть состояния со строго нулевой энергией $E = 0$, которое, тем не менее, уже относится к непрерывному спектру).

Нулевая мода Обратим внимание - в задаче имеется нулевая мода $\epsilon_0 = 0$, соответствующая основному состоянию на языке квантовой механики. Его «волновая функция» тоже выписывалась на семинаре, и она выглядит как (константа C_0 обеспечит нормировку на единицу; $s = 2$):

$$\psi_0(\tau) = \frac{C_0}{\cosh^s \frac{\omega\tau}{2}}$$

В действительности же, наличие нулевой моды, как мы сказали выше, связано с свободой выбора центра инстантона. Это утверждение можно формализовать: $S\left[x_{cl}(\tau)\right] \equiv S\left[x_{cl}(\tau + \delta\tau)\right]$, поэтому инфинитезимальная $\delta\tau$ соответствует «приращению» $z(\tau) = \delta\tau \frac{\partial x_{cl}(\tau)}{\partial \tau}$. С другой стороны,

$$S\left[x_{cl}(\tau) + z(\tau)\right] \approx S\left[x_{cl}(\tau)\right] + S_2[z(\tau)] = S\left[x_{cl}(\tau)\right] + \delta\tau^2 \cdot S_2\left[\frac{\partial x_{cl}}{\partial \tau}\right]$$

и тем самым мы понимаем, что $\frac{\partial x_{cl}}{\partial \tau}$ (с точностью до нормировки) даёт нулевую моду действия S_2. Несложно убедиться, что она (с точностью до константы) совпадает с выписанной тут $\psi_0(\tau)$. В дальнейшем нам приходится нормированное выражение для $\psi_0(\tau)$; это можно сделать в общем виде, используя выражения для действия на инстантоне (11.42). Тем самым, мы получаем:

$$\psi_0(\tau) = \frac{1}{\sqrt{S_0}} \frac{\partial x_{cl}}{\partial \tau}$$

Непрерывный спектр В том-же 4 семинаре исследовался также и непрерывный спектр оператора. В частности, имелось выражение для волновых функций задачи рассеяния (волна падает слева направо - для полного набора к ним, конечно же, нужно добавить также решения, соответствующие падению волны справа налево). Особенностью данного потенциала является то, что при целом s рассеяния оказывается безотражательным, и волновая функция задачи рассеяния содержит только прошедший «кусок».

Непрерывный спектр параметризуется волновым вектором k, так что энергия $E_k = \frac{k^2}{2m} = k^2 \Rightarrow \epsilon_k = \omega^2 + k^2$; а сами волновые функции имеют следующий вид:

$$\psi_k(x) \approx \begin{cases} \frac{\Gamma(1-ika)\Gamma(-ika)}{\Gamma(-ika-s)\Gamma(-ika+s+1)} e^{ikx} \equiv e^{ikx+i\delta(k)} & x \to -\infty \\ e^{ikx}, & x \to +\infty \end{cases}$$

(безотражательность рассеяния означает, что амплитуда прохождения сводится к чистой фазе: $t = e^{-\imath\delta_k}$). Аналитическое выражение для фазы тоже можно выписать (подставляя $a = \frac{2}{\omega}$ и $s = 2$)[6]:

$$e^{-i\delta(k)} = \frac{\Gamma(-ika-2)\Gamma(-ika+3)}{\Gamma(1-ika)\Gamma(-ika)} = \frac{(2-ika)(1-ika)}{(2+ika)(1+ika)} = \frac{1-\frac{ik}{\omega}}{1+\frac{ik}{\omega}} \cdot \frac{1-\frac{2ik}{\omega}}{1+\frac{2ik}{\omega}} = \exp\left(-2i\left[\arctan\frac{k}{\omega} + \arctan\frac{2k}{\omega}\right]\right)$$

$$\delta(k) = 2\left[\arctan\frac{k}{\omega} + \arctan\frac{2k}{\omega}\right] = \begin{cases} 0, & k = 0 \\ 2\pi, & k \to \infty \end{cases}$$

Помимо таких состояний, имеются также и комплексно-сопряжённые решения $\psi^*(x)$, которые описывают волны, падающие справа налево; и вместе они образуют полный набор.

Дискретизация непрерывного спектра В действительности же тут пора вспомнить о том, что на языке функционального интеграла мы рассматриваем траектории на

конечном, хоть и большом, интервале β с нулевыми граничными условиями. Поэтому непрерывный спектр в действительности является дискретным - нам необходимо лишь составить линейную комбинацию ψ_k и ψ_k^*, которая занулялась бы на обоих стенках. Те k, при которых это возможно, и будут давать уровни энергии $\epsilon_n = \omega^2 + k_n^2$. Итак, пусть волновая функция имеет вид $\psi_n(x) = A\psi_k(x) + B\psi_k^*(x)$. Тогда имеется пара условий:

$$\begin{cases} A\psi_k(-\beta/2) + B\psi_k^*(-\beta/2) & = 0 \\ A\psi_k(\beta/2) + B\psi_k^*(\beta/2) & = 0 \end{cases}$$

Такая система уравнений на A и B совместна и имеет ненулевое решение только если её определитель равен нулю:

$$\det \begin{vmatrix} \psi_k(-\beta/2) & \psi_k^*(-\beta/2) \\ \psi_k(\beta/2) & \psi_k^*(\beta/2) \end{vmatrix} = 0$$

Используя асимптотики волновой функции на $\pm\infty$ (известные из задачи рассеяния) мы тем самым получаем:

$$\det \begin{vmatrix} e^{-ik\beta/2+i\delta(k)} & e^{ik\beta/2-i\delta(k)} \\ e^{ik\beta/2} & e^{-ik\beta/2} \end{vmatrix} = 0 \Leftrightarrow \sin(k\beta + \delta(k)) = 0$$

Тем самым, имеется набор k_n, которые являются решением следующего трансцендентного уравнения:

$$k_n\beta - \delta(k_n) = \pi n$$

Обратим внимание, что случаю $n = 0$ соответствует тривиальное решение этого, вообще говоря, трансцендентного уравнения: $k = 0$. Такая волновая функция - тождественный ноль, и нас не интересует. Поэтому нумерация n начинается с 1.

Давайте исследуем, как устроены решения этого уравнения. Вообще говоря, поскольку $\beta \gg 1$ - очень большое число, то при $n \ll \beta$ решения этого уравнения очень близки к $k_n \approx p_n \equiv \frac{\pi n}{\beta}$; поправки можно найти по теории возмущений. С другой стороны, при $n \gtrsim \beta$, фазы рассеяния уже выходят на константу $\delta(k_n) \approx \delta(k_n \to \infty) = 2\pi$. Поэтому решение уравнения устроены следующим образом:

$$k_n \approx p_n + \delta(p_n)/\beta, \quad p_n = \pi n/\beta$$

Нормировка функционального интеграла

11.4.8 Нормировка функционального интеграла Конечно, как мы уже обсуждали ранее, мера функционального интеграла $\mathcal{D}$ содержит бесконечную константу $\mathcal{N}$, связанную с дискретизацией - и поэтому буквально выписанным выражением воспользоваться не удастся. Для того, чтобы придать этому выражению смысл, необходимо рассмотреть отношение двух функциональных интегралов, в котором эта бесконечная нормировка сократится. В качестве такого выражения удобно использовать уже сосчитанную ранее функцию Грина квантового гармонического осциллятора; удобно выбрать его с такой же частотой ω, чтобы квадратичные операторы, стоящие в действии были похожи:

Спектр оператора (знаменатель)

$$G_0(\beta) = \int\limits_{z(-\beta/2)=0}^{z(\beta/2)=0} \mathcal{D}[z(\tau)] \exp\left(-\frac{1}{2}\int\limits_{-\beta/2}^{\beta/2} \left[(\partial_\tau z)^2 + \omega^2 z^2\right]\right) = \sqrt{\frac{\omega}{2\pi \sinh \omega\beta}}$$

И тем самым мы, в действительности, будем работать со следующим выражением:

$$\frac{G(\eta,-\eta,\beta)}{G_0(\beta)} = e^{-S_0}\frac{\int\limits_{z(-\beta/2)=0}^{z(\beta/2)=0}\mathcal{D}[z(\tau)]\exp\left(-\frac{1}{2}\int\limits_{-\beta/2}^{\beta/2}d\tau\left[(\partial_\tau z)^2+U''\left(x_{cl}(\tau)\right)z^2(\tau)\right]\right)}{\int\limits_{z(-\beta/2)=0}^{z(\beta/2)=0}\mathcal{D}[z(\tau)]\exp\left(-\frac{1}{2}\int\limits_{-\beta/2}^{\beta/2}d\tau\left[(\partial_\tau z)^2+\omega^2 z^2\right]\right)}$$

11.4.9 Спектр оператора (знаменатель) Собственно, с функциональным интегралом, что стоит в знаменателе, мы уже работали - поэтому кратко озвучим результаты. В принципе, оператор $(-\partial_\tau^2+\omega^2)$, который там стоит, тоже похож на уравнение Шрёдингера в константном потенциале $U(\tau)=\omega^2=\text{const}$, и тоже обладает лишь непрерывным спектром. Однако нулевые граничные условия, как и в прошлый раз, спектр дискретизуют, волновые функции $\psi_k^{(0)}(\tau)$ представляют собой стоячие волны, а спектр получается следующий:

$$\epsilon_p^{(0)}=\omega^2+p^2,\quad p=p_n=\pi n/\beta$$

Вычисление гауссового интеграла

11.4.10 Вычисление гауссового интеграла Итак, мы вплотную приблизились к тому, чтобы, наконец, посчитать гауссов функциональный интеграл. Мы делаем разложение в числителе вида $z(\tau)=\sum\limits_n c_n\psi_n(\tau)$ (учитывая дискретный спектр!) и в знаменателе $z(\tau)=\sum\limits_n c_n\psi_n^{(0)}(\tau)$. Учитывая гауссовость обоих интегралов, мы получаем:

$$\frac{G(\eta,-\eta,\beta)}{G_0(\beta)} = e^{-S_0}\prod_n\left(\frac{\int dc_n\exp\left(-\frac{1}{2}\epsilon_n c_n^2\right)}{\int dc_n\exp\left(-\frac{1}{2}\epsilon_n^{(0)}c_n^2\right)}\right)$$

Нулевая мода Итак, интеграл по dc_0, соответствующий нулевой моде $\psi_n(\tau)$, происходит в бесконечных пределах, выглядит как $\int dc_0$ и в гауссовом приближении расходится - в таком случае, как правило, интеграл нужно брать точно. Наличие нулевых мод, как правило, связаны с какой-то симметрией - в данном случае, трансляционной; и в таком случае интегрирование обычно сводится к объёму соответствующей группы симметрии.

В нашем случае, нулевая мода напрямую связана с произвольностью выбора константы τ_c в инстантоне, который имеет вид $x_c(\tau-\tau_c)$. Заметим, что смещение вдоль нулевой моды dc_0 в точности соответствует смещению центра инстантона:

$$d\left(x_{cl}(\tau-\tau_c)\right)\equiv\psi_0(\tau)dc_0,\quad d\left(x_{cl}(\tau-\tau_c)\right)\equiv\frac{\partial x_{cl}}{\partial\tau}d\tau_c$$

Приравнивая эти два выражения, и замечая, что $\psi_0(\tau)=\frac{1}{\sqrt{S_0}}\frac{\partial x_{cl}}{\partial\tau}$, мы получаем следующий вид интеграла по нулевой моде в числителе: $\int dc_0\equiv\sqrt{S_0}\int d\tau_c=\beta\sqrt{S_0}$. В соответствующем выражении в знаменателе стоит следующий интеграл (там нумерация n начинается с 1, что, впрочем, не очень важно - ведь мы имеем дело с непрерывным спектром, и все собственные числа с маленькими номерами малы):

$$\int dc_1 e^{-\frac{1}{2}\epsilon_1^{(0)}c_1^2}=\sqrt{\frac{2\pi}{\epsilon_1^{(0)}}}=\sqrt{\frac{2\pi}{\omega^2+\pi^2/\beta^2}}\underset{\beta\to\infty}{\approx}\frac{\sqrt{2\pi}}{\omega}$$

Тем самым, если ввести условное обозначение $\det' \hat{L}$ - интеграл с исключённым наименьшим собственным числом то бишь отщепив нулевую моду - мы получаем:

$$\frac{G(\eta,-\eta,\beta)}{G_0(\beta)} = e^{-S_0} \cdot \left(\omega\beta\sqrt{\frac{S_0}{2\pi}}\right) \cdot \left(\frac{\det'\left(-\partial_\tau^2 + U''\left(x_{cl}(\tau)\right)\right)}{\det'\left(-\partial_\tau^2+\omega^2\right)}\right)^{-1/2}$$

Возникновение множителя $\sqrt{S_0}$, связанного с нулевой модой - утверждение в действительности совершенно общего характера.

Дискретный спектр Помимо нулевой моды, имеется также ещё одно состояние дискретного спектра, $\epsilon_1 = \frac{3}{4}\omega^2$. Оно даст следующий вклад (отнормированный на соответствующий вклад $\epsilon_2^{(0)} = \omega^2 + (2\pi/\beta)^2 \approx \omega^2$ от осциллятора:

$$\frac{\epsilon_1}{\epsilon_2^{(0)}} \underset{\beta\to\infty}{\approx} \frac{\frac{3}{4}\omega^2}{\omega^2} = \frac{3}{4}$$

Непрерывный спектр Итак, самое сложное - вычисление состояния непрерывного спектра, бесконечного произведения (обратите внимание, нумерация в числителе начинается с $n=1$, а в знаменателе - с $n=3$, поскольку первых два состояния мы уже «отщепили» при работе с дискретным спектром). Для вычисления, это бесконечное произведение удобно прологарифмировать, а также воспользоваться приближенным решением трансцедентного уравнения $k_n \approx p_n - \delta\left(p_n\right)/\beta$:

$$\begin{aligned}
\frac{\det''}{\det''} &= \prod_{n=1}^{\infty} \frac{\omega^2+k_n^2}{\omega^2+p_{n+2}^2} = \\
&= \exp\left(\sum_{n=1}^{\infty} \ln\frac{\omega^2+k_n^2}{\omega^2+p_{n+2}^2}\right) = \\
&= \exp\left(\sum_{n=1}^{\infty} \ln\left(1+\frac{k_n^2-p_{n+2}^2}{\omega^2+p_{n+2}^2}\right)\right) \approx \exp\left(\sum_{n=1}^{\infty}\frac{k_n^2-p_{n+2}^2}{\omega^2+p_{n+2}^2}\right) \approx \\
&\approx \exp\left(\sum_{n=1}^{\infty}\frac{2p_{n+2}\left(k_n-p_{n+2}\right)}{\omega^2+p_{n+2}^2}\right) = \qquad\qquad = \exp\left(\frac{1}{\beta}\sum_{n=1}^{\infty}\frac{\left(\delta\left(p_n\right)-2\pi\right)2p_{n+2}}{\omega^2+p_{n+2}^2}\right)
\end{aligned}$$

Вообще говоря, тот факт, что k_n и p_n очень близки (по $\frac{1}{\beta}$) на всём промежутке произведения означает, что все члены произведения очень близки к 1, и только за счёт их большого количества ($\sim\beta$) это произведение оказывается отличным от единицы (а сумма - от нуля). Для суммирования плавной функции, удобно заменить сумму на интеграл, согласно $\sum\limits_n = \int\limits_0^\infty \frac{\beta dp}{\pi}$ и увидеть, что β из ответа полностью выпадает, а ответ - конечный:

$$\frac{\det''}{\det''} = \exp\left(\int_0^\infty \frac{dp}{\pi}\frac{2p(\delta(p)-2\pi)}{\omega^2+p^2}\right)$$

Обратим внимание, что полученный тут член 2π обеспечивает сходимость интеграла на бесконечности (ведь $\delta(p\to\infty)\to 2\pi$); в противном случае интеграл бы логарифмически расходится. Само число 2π явно связано с количеством связанных состояний; но ровно с этим же и связана фаза $\delta(p\to\infty)$! - поэтому теорема Левинсона, о которой сказано в примечании, в действительности гарантирует сходимость этого интеграла на бесконечности. Следующий шаг - интегрирование по частям:

$$\frac{\det''}{\det''} = \exp\left(-\frac{1}{\pi}\int_0^\infty dp\frac{d\delta}{dp}\ln\frac{\omega^2+p^2}{\omega^2}\right)$$

Прелесть этого выражения ещё и в том, что этот неприятный 2π-член, который «помнит» о количестве связанных состояний, в него не входит; а кроме того, фаза - вообще говоря, многозначная функция, и плохо определена (с точностью до $2\pi n$), а вот производная фазы определена уже хорошо. Поэтому, например, в инстантонной азбуке не сильно «заморачиваются» с явным выражением для фазы и отделением этого 2π-члена, а приходят к этому выражению, с которым уже и работают. Итак, оставшийся интеграл обезразмеривается подстановкой $p = \omega y$, считается явно и даёт:

$$\int\limits_0^\infty dp \frac{d\delta}{dp} \ln\left(1+\frac{p^2}{\omega^2}\right) = 2\int\limits_0^\infty dy \ln\left(1+y^2\right)\left[\frac{1}{y^2+1}+\frac{2}{4y^2+1}\right] = 2\pi\ln 3$$

а вклад от непрерывного спектра равен:

$$\frac{\det''}{\det''} = \frac{1}{9}$$

Одноинстантонный ответ

Во-первых, тем самым мы получили ответ для отношения детерминантов (с исключённой нулевой модой):

$$\frac{\det'\left(-\partial_\tau^2+\omega^2-\frac{3\omega^2/2}{\cosh^2(\omega\tau/2)}\right)}{\det'\left(-\partial_\tau^2+\omega^2\right)} = \frac{3}{4}\cdot\frac{1}{9} = \frac{1}{12}$$

и мы получили следуюгцй ответ (в одноинстантонном приближении):

$$\frac{G(\eta,-\eta,\beta)}{G_0(\beta)} = e^{-S_0}\cdot\underbrace{\left(\omega\beta\sqrt{\frac{S_0}{2\pi}}\right)}_{\text{zero mode}}\cdot\underbrace{\sqrt{\frac{4}{3}}}_{\text{bound state}}\cdot\underbrace{\sqrt{9}}_{\text{continuous spectrum}} = \sqrt{\frac{6}{\pi}S_0}\omega\beta e^{-S_0}$$

Наличие тут явной зависимости от бесконечной величины β должно смущать - ведь мы рассматриваем предел $\beta\to\infty$. В действительности же этот ответ, как инстантонная поправка, получен в пределе, покуда он мал $-\sqrt{S_0}\omega\beta e^{-S_0} \ll 1$ - и поэтому буквально бесконечной β сделать не удастся. С другой стороны, от β он явно зависит не экспоненциальным образом, поэтому пока непонятно, как извлечь из него непосредственно туннельное расщепление.

В действительности же найденный ответ - это первый порядок разложения по e^{-S_0}. Настоящий же ответ устроен попросту как

$$\frac{G(\eta,-\eta,\beta)}{G_0(\beta)} = \sinh(\Delta\beta), \quad \Delta = \omega\cdot\sqrt{\frac{6S_0}{\pi}}e^{-S_0} = \frac{2}{\sqrt{\pi}}\omega\cdot\sqrt{\omega\eta^2}e^{-2\omega\eta^2/3}.$$

То, что ответ должен быть таким, само по себе достаточно очевидно - мы знаем, что в реальном времени если посадить частицу в одну из ям, то она будет испытывать осцилляции Раби $\sin(\Delta t)$, и Δ даётся как раз туннельным расщеплением симметричного и антисимметричного состояния. В мнимом же времени, экспоненциальная зависимость восстанавливается; рассматривая разложения по собственным модам вида $G(x,y,\beta) = \sum\limits_n \psi_n(x)\psi_n^*(y)e^{-\beta E_n}$, мы немедленно понимаем, что в задаче имеется пара уровней энергии $E = \frac{\omega}{2}\pm\Delta$. Тем не менее, чтобы получить этот ответ систематически, необходимо уйти за рамки одноинстантонного приближения, и рассмотреть многоинстантонные вклады.

Разреженный инстантонный газ

Помимо найденной единственной траектории $x_{cl}(\tau)$, при которой частица перекатывается из одного «горба» перевёрнутого потенциала на другой, имеются также и траектории, в которых она многократно катается «туда-сюда» (см. рис.).

Давайте выясним, как устроен вклад от таких траекторий в приближении, что инстантоны расположены достаточно далеко друг от друга (это приближение носит название приближения разреженного инстантонного газа; ниже мы выясним, какому параметру оно соответствует). Во-первых, действие на такой траектории из n инстантонов, очевидным образом, будет равно $S_n = nS_0$, а эффективный потенциал с экспоненциальной точностью устроен как набор аналогичных ям от каждого инстантона. Интуитивно понятно, что и квадратичные флуктуации вблизи каждого инстантона факторизуются,'

поскольку инстантоны достаточно хорошо разнесены в пространстве [7]; это можно показать и явно. В каждой из ям будет свой набор состояний дискретного спектра, поэтому вклад от последнего факторизуется. Непрерывный же спектр устроен безотражательно для каждого из инстантонов - поэтому полная фаза рассеяния на всех инстантонах будет попросту суммой фаз от каждого из инстантонов, $\delta^{(n)}(p) = n\delta(p)$ - из-за чего факторизуется также и вклад от непрерывного спектра. Наконец, с каждым из инстантонов будет связана своя нулевая мода - интегрирование по положению его центра; и вклад от нулевых мод будет устроен следующим образом:

$$\int\limits_{-\beta/2<\tau_1<\tau_2<\cdots<\tau_n<\beta/2} d\tau_1 ... d\tau_n = \frac{\beta^n}{n!}$$

Для перехода $-\eta \to \eta$, только конфигурации с нечётным количеством инстантонов дают вклад. Поэтому, суммирование разреженного инстантонного газа приводит к следующему ответу:

$$\frac{G(\eta, -\eta, \beta)}{G_0(\beta)} = \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} \left(\sqrt{\frac{6}{\pi} S_0} \omega \beta e^{-S_0} \right)^{2n+1} = \sinh \left(\sqrt{\frac{6}{\pi} S_0} \omega \beta e^{-S_0} \right)$$

Точно такое же суммирование можно было бы провести и для, например, $\eta \to \eta$. В таком случае очевидным образом вклад давали бы только конфигурации с чётным количеством инстантонов, и в ответе ожидаемым образом получился бы cosh.

Давайте выясним, по какому параметру работает наше приближение. Мы имеем дело с суммой $\sum\limits_{n=0}^{\infty} \frac{(\Delta\beta)^{2n+1}}{(2n+1)!}$. Члены этого ряда с n сначала возрастают (из-за, вообще говоря, большого множителя $\Delta\beta$), а затем убывают (из-за факториала в знаменателе - ряд-то сходится!). Можно убедиться, что пик приходится на $n^* \approx \Delta\beta$, и именно такие инстантонные конфигурации дают наибольший вклад в сумму, и условие разреженности должно выполняться именно для них. С другой стороны, типичная ширина каждого инстантона равна, как мы помним, ω^{-1}; требование сводится к тому, что ширина n^* инстантонов должна быть по-прежнему маленькой по сравнению со всей длиной отрезка β. Этот критерий соответствует $\Delta \ll \omega$; тем самым, наше приближение работает только покуда инстантонная поправка является маленькой (что совершенно ожидаемо) - это, в свою очередь, соответствует туннельному пределу $S_0 \gg 1$.

Формализм Гельфанда - Яглома

На прошлом семинаре мы столкнулись с необходимостью вычисления функциональных детерминантов операторов типа Шрёдингера. Для его вычисления нам

потребовалось найти собственные значения дискретного, и волновые функции непрерывного спектра, а затем вычислять бесконечные произведения. В задаче прошлого семинара мы смогли с этим справиться из-за наличия точного решения потенциала в терминах гипергеометрической функции. С другой стороны, в более сложных приложениях такого решения может не существовать, и возможно, детерминант придётся находить численно - и достаточно очевидно, что изложенный выше способ непригоден для численного анализа. В данном семинаре будет изложен альтернативный и достаточно красивый способ, который позволяет найти ответ значительно проще.

Дискретная формулировка и доказательство

Допустим, мы хотим найти «характеристический многочлен» $f(\lambda) = \det(\hat{H} - \lambda)$, где $\hat{H} = -\partial_x^2 + U(\hat{x})$ - какой-то квантомеханический гамильтониан (забудем пока на время о бесконечных нормировочных константа и что сам детерминант, вообще говоря, определён плохо). Чтобы определить задачу полностью, помимо оператора, нам также необходимо задать класс функций, на которых он действует - например, функции, заданные на отрезке с бесконечными стенками $\psi(0) = \psi(L) = 0$. Дискретизуем пространство с шагом ϵ; матрицу $\hat{H}$ в таком случае можно задать совершенно явно $(x_k = k \cdot \epsilon, \epsilon = L/(N+1), \psi_0 = 0)$

$$\left(\hat{H}_N \psi\right)_n = -\frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{\epsilon^2} + U(x_n)\,\psi_n,$$

$$\hat{H}_N = \frac{1}{\epsilon^2}\begin{pmatrix} 2+\epsilon^2 U(x_1) & -1 & 0 & ... & 0 & \\ -1 & 2+\epsilon^2 U(x_2) & -1 & \cdots & 0 & \\ 0 & -1 & 2+\epsilon^2 U(x_3) & \ddots & \vdots & \\ \vdots & \vdots & \ddots & \ddots & -1 & \\ 0 & 0 & & ... & -1 & 2+\epsilon^2 U(x_N) \end{pmatrix}$$

(и задача становится хорошо определённой). Обозначим $f_N(\lambda) = \det\left(\hat{H}_N - \lambda\right)$; чуть удобнее будет вынести ϵ^{-2}, как на формуле выше, вычислить определитель оставшейся матрицы $g_N(\lambda) = \epsilon^{2N} f_N(\lambda)$. Не мудрствуя лукаво, давайте распишем оставшийся определитель по последней строчке; тем самым он свяжется с определителями подматрицы на один и два размера меньше рекуррентным соотношением [8]:

$$g_{N+1} = \left(2 + \epsilon^2\left(U(x_{N+1}) - \lambda\right)\right) g_N - (-1)(-1) g_{N-1} \Rightarrow -\frac{g_{N+1} - 2g_N + g_{N-1}}{\epsilon^2} + \left(U(x_{N+1}) - \lambda\right) g_N = 0$$

Возвращаясь к непрерывному пределу $g_N(\lambda) = g(x = N\epsilon|\lambda)$, мы немедленно видим нетривиальный факт - сам определитель удовлетворлет такому уравнению Шрёдингера! В этом - суть теоремы Гельфанда-Яглома, и это уже хороший рецепт нахождения определителя - осталось лишь добавить начальные условия. В дискретном представлении они следующие:

$$g_1(\lambda) = 2 + \epsilon^2 U(x_1) \approx 2, \quad g_2(\lambda) = \left(2 + \epsilon^2 U(x_1)\right)\left(2 + \epsilon^2 U(x_2)\right) - 1 \approx 3,$$

что означает, что в непрерывном пределе функция $\psi(x|\lambda) = \epsilon g(x|\lambda)$ имеет хорошо определённые граниченые условия. Тем самым, в пределе $\epsilon \to 0$ задача решается следующим образом:

$$\det\left(\hat{H}_N - \lambda\right) = \frac{1}{\epsilon^{2N-1}}\psi(L = N\epsilon|\lambda), \quad \hat{H}\psi(x|\lambda) = \lambda\psi(x|\lambda), \quad \psi(0|\lambda) = 0, \quad \partial_x\psi(0|\lambda) = 1$$

Вместо нахождения всех решений краевой задачи $\psi(0) = \psi(L) = 0$, нам необходимо решить одну единственную эволюционную задачу (как в «методе стрельбы») - это существенное упрощение. Как обычно, чтобы кроме того избавиться от всевозможных бесконечных нормировочных констант, связанных с дискретизацией, мы можем рассмотреть отношение двух детерминантов - которое уже определено хорошо:

$$\frac{\det\left(\hat{H}_1 - \lambda\right)}{\det\left(\hat{H}_2 - \lambda\right)} = \frac{\psi_1(L|\lambda)}{\psi_2(L|\lambda)}$$

Теперь давайте обсудим полученный результат. Во-первых, выбрать граничное условие $\partial_x\psi$ можно любым - лишь бы для обоих волновых функций $\psi_{1,2}$ оно было выбрано одинаковым. Во-вторых, полученный результат непосредственно обобщается и на более сложные операторы, например, на уравнение Шрёдингера в двух или трёх измерениях (где оператор, задающий уравнение волновую функцию устроено не буквально как $-\partial_x^2 + U(x)$). Предложенные тут правдоподобные рассуждения как вариант доказательства теоремы Гельфанда-Яглома не единственные - вообще говоря, к тому же результату можно было бы прийти иначе. А именно, можно заметить, что если $\psi(0|\lambda) = 0$, то $\psi(L|\lambda) = 0$ тогда и только тогда, когда λ является собственным числом оператора $\hat{H}$ - а это, в свою очередь, означает, что нули функций $\det(\hat{H} - \lambda)$ и $\psi(L|\lambda)$ как функции переменной λ совпадают. Из ТФКП известно, что эти функции в таком случае могут отличаться лишь на какую-то целую функцию - и эта целая функция для числителя и знаменателя оказывается одинаковой, если выбраны одинаковые граничные условия задачи «стрельбы» $\partial_x\psi(0|\lambda)$. Поэтому полученная тут связь совершенно неудивительна, и её стоило бы ожидать.

Пример: осциллятор

Давайте рассмотрим в качестве примера простой гармонический осциллятор в мнимом времени, $\hat{H}_1 = -\partial_\tau^2 + \omega^2$; а в качестве знаменателя возьмём свободную частицу, $\hat{H}_2 = -\partial_\tau^2$; положим $\lambda = 0$ (такую задачу в реальном времени мы решали два семинара назад, когда только учились брать гауссовы интегралы). Решения соответствующих эволюционных задач записываются устно:

$$\left(-\partial_\tau^2 + \omega^2\right)\psi_1(x) = 0 \Rightarrow \psi_1(\tau) = \frac{\sinh\omega\tau}{\omega}$$
$$-\partial_\tau^2\psi_2(x) = 0 \Rightarrow \psi_2(\tau) = \tau$$

и значит, для функций, заданных на отрезке длины β, отношение определителей равно:

$$\frac{\det\hat{H}_1}{\det\hat{H}_2} = \frac{\sinh\omega\beta}{\omega\beta}$$

Тот же результат получался и ранее с нахождением спектра, что было несколько сложнее.

Пример: флуктуации вблизи инстантона

Теперь давайте перейдём к примеру сложнее - а именно, рассмотрим оператор $\hat{H}_s = -\partial_x^2 - \frac{s(s+1)}{\cosh^2 x}$. Именно с таким оператором ($s = 2$) мы имели дело на прошлом семинаре. Обозначим также $\lambda = -\kappa^2$. Нам нужно решать задачу стрельбы; сразу заметим, что поскольку $\lambda < 0$, то уравнение Шрёдингера решается на отрицательных

энергиях, поэтому решения непременно будут экспоненциально растущими. Нормировать мы будем на осциллятор - такой же оператор, но с $s = 0$. Наконец, поскольку мы рассматриваем задачу на отрезке $(-L, L)$, то удобно воспользоваться симметрией задачи относительно инверсии. Как мы знаем, эта симметрия означает, что все собственные волновые функции можно выбрать либо чётными, либо нечётными - а значит, и в определитель будет вклад как от чётных, так и от нечётных мод, и эти вклады разделяются. Поэтому и мы тоже можем искать отдельно отношение определителей, вычисленных по чётным и по нечётным состояниям - для этого можно «стрелять» не из $x = -\beta/2$, а из нуля $x = 0$, и решать следующие две задачи («+» и «-» соответствуют чётным и нечётным решениям):

Давайте теперь решать уравнение Шрёдингера. Конечно, без гипергеометрической функции не обойтись - УШ ведь получается таким же. Для поиска чётных и нечётных решений удобно воспользоваться заменой переменных $y = \cosh^2 x$, которая приводит УШ к следующему виду:

$$y(1-y)\psi''(y) + \left(\frac{1}{2} - y\right)\psi'(y) - \left(\frac{s(s+1)}{4y} - \frac{\kappa^2}{4}\right)\psi(y) = 0$$

Подстановка $\psi(y) = y^{(s+1)/2}\chi(y)$ приводит его к гипергеометрическому виду:

$$y(1-y)\chi''(y) + \left[\left(s + \frac{3}{2}\right) - y(s+2)\right]\chi'(y) - \left(\frac{(s+1)^2 - \kappa^2}{4}\right)\chi(y) = 0,$$

однако чуть проще оно записывается для переменной $z = 1 - y = -\sinh^2 x$:

$$z(1-z)\chi''(z) + \left[\frac{1}{2} - z(s+2)\right]\chi'(z) - \left(\frac{(s+1)^2 - \kappa^2}{4}\right)\chi(z) = 0.$$

Сравнивая полученное уравнение с уравнением для гипергеометрической функции, мы немедленно получаем следующие значения параметров:

$$a = \frac{s+1+\kappa}{2}, \quad b = \frac{s+1-\kappa}{2}, \quad c = \frac{1}{2},$$

а также общий вид решения в виде линейной комбинации ${}_2F_1(a, b; c; z)$ и $z^{1-c}{}_2F_1(b-c+1, a-c+1; 2-c; z)$; для исходных функций решения имеют следующий вид:

$$\begin{cases} \psi^{(+)}(x) = \cosh^{s+1} x \cdot {}_2F_1\left(\frac{s+1+\kappa}{2}, \frac{s+1-\kappa}{2}; \frac{1}{2}; -\sinh^2 x\right) \\ \psi^{(-)}(x) = \sinh x \cdot \cosh^{s+1} x \cdot {}_2F_1\left(\frac{s-\kappa+2}{2}, \frac{s+\kappa+2}{2}; \frac{3}{2}; -\sinh^2 x\right) \end{cases}$$

Выбранные таким образом, они удовлетворяют необходимым граничным условиям: $\psi^{(+)}(x \ll 1) \approx 1$ и $\psi^{(-)}(x \ll 1) \approx x$. Асимптотики (бесконечность) Мы хотим найти определитель для системы со стенками, расположенными достаточно далеко $\kappa L \gg 1$, поэтому нам необходимо найти далёкие асимптотики функций $\psi^{(\pm)}(x \to \infty)$ (которые, напомним, должны быть экспоненциально возрастающими, поскольку мы имеем дело с движением на отрицательной энергии). Для того, чтобы найти асимптотику гипергеометрической функции, нам необходимо воспользоваться одной из многих формул преобразования аргумента в данном случае, $z \mapsto \frac{1}{z}$ (который переводит ∞ в 0, а асимптотика в нуле уже хорошо известна). Преобразование имеет следующий вид:

$${}_2F_1(a, b; c; z) = \frac{\Gamma(c)\Gamma(b-a)}{\Gamma(b)\Gamma(c-a)}\frac{1}{(-z)^a}\cdot{}_2F_1\left(a, 1-c+a; 1-b+a; \frac{1}{z}\right) + \frac{\Gamma(c)\Gamma(a-b)}{\Gamma(a)\Gamma(c-b)}\frac{1}{(-z)^b}\cdot{}_2F_1\left(b, 1-c+b;\right.$$

Сами гипергеометрические функции дают асимптотику ${}_2F_1(...,0) \approx 1$; для функции $\psi^{(+)}$значение $a > b$, из-за чего важнее оказывается второе слагаемое; а для $\psi^{(-)}$—наоборот, первое. Асимптотики получаются следующими:

$$\begin{cases} \psi^{(+)}(x) \approx \frac{\Gamma(1/2)\Gamma(\kappa)}{\Gamma((s+1+\kappa)/2)\Gamma((\kappa-s)/2)} \coth^{s+1} x \cdot \sinh^{\kappa} x \approx \frac{\Gamma(1/2)\Gamma(\kappa)}{2^{\kappa}\Gamma((1+s+\kappa)/2)\Gamma((\kappa-s)/2)} e^{\kappa x} \\ \psi^{(-)}(x) \approx \frac{\Gamma(3/2)\Gamma(\kappa)}{\Gamma((s+\kappa+2)/2)\Gamma((1-s+\kappa)/2)} \coth^{s+1} x \sinh^{\kappa} x = \frac{\Gamma(3/2)\Gamma(\kappa)}{2^{\kappa}\Gamma((s+\kappa+2)/2)\Gamma((1-s+\kappa)/2)} e^{\kappa x} \end{cases}$$

В знаменателе же стоит решение задачи в отсутствии потенциала («квантовый гармонический осциллятор» в терминах исходной задачи, или свободная частица в терминах соответствующего УШ), который мы уже выписывали ранее:

$$\begin{cases} \psi_0^{(+)}(x) = \cosh \kappa x \approx e^{\kappa x}/2 \\ \psi_0^{(-)}(x) = \sinh \kappa x/\kappa \approx e^{\kappa x}/2\kappa \end{cases}$$

Тем самым, отношение определителей принимает следующий вид:

$$\frac{\det\left(\hat{H}_s + \kappa^2\right)}{\det\left(\hat{H}_0 + \kappa^2\right)} = \frac{2\Gamma(1/2)\Gamma(\kappa)}{2^{\kappa}\Gamma((1+s+\kappa)/2)\Gamma((\kappa-s)/2)} \cdot \frac{2\kappa\Gamma(3/2)\Gamma(\kappa)}{2^{\kappa}\Gamma((s+\kappa+2)/2)\Gamma((1-s+\kappa)/2)}$$

$$= \frac{\pi\kappa\Gamma^2(\kappa)}{2^{2\kappa-1}\Gamma((1+s+\kappa)/2)\Gamma((\kappa-s)/2)\Gamma((s+\kappa+2)/2)\Gamma((1-s+\kappa)/2)}$$

'Полученный ответ можно ещё упростить, используя соотношение $\Gamma(x)\Gamma(x+1/2) = \sqrt{\pi}\Gamma(2x)/2^{2x-1}$. Окончательно, имеем:

$$\frac{\det\left(\hat{H}_s + \kappa^2\right)}{\det\left(\hat{H}_0 + \kappa^2\right)} = \frac{\kappa\Gamma^2(\kappa)}{\Gamma(1+s+\kappa)\Gamma(\kappa-s)}$$

Применение к инстантону

На прошлом семинаре мы считали следующее отношение определителей:

$$\frac{\det'\left(-\partial_\tau^2 + \omega^2 - 3\omega^2/2\cosh^2(\omega\tau/2)\right)}{\det'\left(-\partial_\tau^2 + \omega^2\right)}.$$

Напомним, штрих в числителе означал, что нужно «убрать» нулевую моду, а в знаменателе - что нужно убрать наинизшую моду. Давайте вычислим его, используя нашу общую формулу.Во-первых, чтобы привести его к нужному виду, необходимо сделать замену $x = \frac{\omega\tau}{2}$:

$$\frac{\det'\left(\frac{\omega^2}{4}\left[-\partial_x^2 + 4 - 6/\cosh^2 x\right]\right)}{\det'\left(\frac{\omega^2}{4}\left[-\partial_x^2 + 4\right]\right)} = \frac{\det'\left(\hat{H}_2 + 4\right)}{\det'\left(\hat{H}_0 + 4\right)}$$

Во-вторых, поскольку оба определителя «штрихованные», то константы можно сократить (собственные числа делятся друг на друга попарно и эти константы попарно же сокращаются - в противном случае, скажем, для отношения вида $\det'/\det$, такая константа могла бы «выскочить» в ответ); значит, мы немедленно получаем $s = 2$ и $\kappa = 2$. Если подставить эти параметры буквально в полученную выше формулу, мы получим ноль (поскольку $(\kappa - s)$ в знаменателе обращается в бесконечность), что

ожидаемо - в формуле штрихи стоят неспроста. В формализме Гельфанда-Яглома выбросить нулевую моду можно достаточно просто: давайте чуть-чуть сместим λ и рассмотрим отношение определителей $\det\left(\hat{H}_2+\ 4+\epsilon\right)/\det\left(\hat{H}_0+4+\epsilon\right)$. В таком случае, нулевая мода станет малой и равной ϵ; остальные же моды изменятся слабо. Добавив также «выброшенную» наименьшую моду в знаменателе, чтобы убрать штрих и оттуда, мы получаем:

$$\frac{\det'\left(\hat{H}_2+4\right)}{\det'\left(\hat{H}_0+4\right)}=\lim_{\epsilon\to 0}\frac{\frac{1}{\epsilon}\det\left(\hat{H}_2+4+\epsilon\right)}{\frac{1}{4}\det\left(\hat{H}_0+4+\epsilon\right)}$$

Теперь мы готовы считать. Подставляем $\kappa^2=4+\epsilon\Rightarrow\kappa=2+\epsilon/4$ и получаем:

$$\frac{\det\left(\hat{H}_2+4+\epsilon\right)}{\det\left(\hat{H}_0+4+\epsilon\right)}\underset{\epsilon\ll 1}{\approx}\frac{2\Gamma^2(2)}{\Gamma(5)\Gamma\left(\frac{\epsilon}{4}\right)}=\frac{\epsilon}{48},$$

и тем самым мы воспроизводим ответ, полученный ранее: $\frac{\det'\left(\hat{H}_2+4\right)}{\det'\left(\hat{H}_0+4\right)}=1/12$.

Инстантоны: распад метастабильного состояния

На этом семинаре мы разберём ещё одну задачу квантовой механики, которая тоже решается при помощи инстантонов и которая тоже имеет туннельную природу. Речь идёт о задаче распада метастабильного состояния (см. семинар 8 прошлого семестра). Хотя технически эта задача очень похожа на задачу о туннельном расщеплении в двухъямном потенциале, в ней есть несколько крайне важных мест, которые стоит обсудить отдельно. Сама задача формулируется следующим образом. Частица массы $m=1$ описывается следующим гамильтонианом:

$$\hat{H}=-\frac{1}{2}\partial_x^2+\lambda x^2(\eta-x)$$

В окрестности $x=0$ имеется локальный минимум, а сам потенциал имеет вид осциллятора с частотой $\omega=\sqrt{2\lambda\eta}$. Если бы этот минимум был бы глобальным, то для низколежащих уровней имелась бы серия стационарных связанных состояний $E_n=\omega\left(n+\frac{1}{2}\right)$. Однако в нашей задаче никаких стационарных состояний нет, имеется только непрерывный спектр - поэтому если частицу поместить на один из этих осцилляторных уровней энергии, то рано или поздно частица протуннелирует через барьер (который мы считаем достаточно высоким, чтобы квазистационарное состояние было хорошо определённым). Как мы обсуждали ранее, такой процесс формально эквивалентен мнимой добавке к уровням энергии $E_n-i\frac{\Gamma_n}{2}$, так что обычная унитарная эволюция для таких состояний будет приводить к экспоненциальному затуханию вероятности со временем $\psi_n\propto e^{-i(E_n-i\Gamma_n/2)t}\Rightarrow|\psi_n|^2\propto e^{-\Gamma_n t}$.

Давайте сперва формально повторим инстантонное вычисление, пропуская важные моменты - а в самом конце обсудим их. 11.6.1

Функциональный интеграл

Итак, мы хотим исследовать функцию Грина, дающую вероятность остаться в яме, $G(0,0,t)=\left\langle 0\left|e^{-i\hat{H}t}\right|0\right\rangle$. В мнимом времени $t=-i\beta$, в эту величину будет давать основной вклад основное состояние [10], и мы получим:

$$G_E(0,0,\beta)\approx\sum_n|\langle 0|n\rangle|^2e^{-\beta E_n+i\beta\Gamma_n/2}\approx|\langle 0|n=0\rangle|^2e^{-\beta E_0+i\beta\Gamma_0/2}$$

С другой стороны, для Евклидовой функции Грина можно записать следующий функциональный интеграл:

$$G_E(0,0,\beta) = \int\limits_{x(-\beta/2)=0}^{x(\beta/2)=0} \mathcal{D}x(\tau) e^{-S_E}, \quad S_E = \int\limits_{-\beta/2}^{\beta/2} d\tau \left(\frac{1}{2} \left(\partial_\tau x\right)^2 + U(x) \right)$$

Как обычно, Евклидово действие представляет собой обычное действиие, но в перевёрнутом потенциале [11], имеющим вид, изображённый на рисунке.

Инстантон

Следуя пройденному ранее пути, нам необходимо найти инстантон (в пределе $\beta \to \infty$) - седловую траекторию, дающую экстремум действия S_E. Как обычно, мы будем это делать, используя первый интеграл:

$$\partial_\tau^2 x = U'(x) = \lambda x(2\eta - 3x), \quad E = \frac{1}{2}\left(\partial_\tau x\right)^2 - U(x) = 0 \Rightarrow \partial_\tau x = \sqrt{2U(x)}$$

Имеются тривиальные траектории $x = 0$ (которая даст нам осцилляторные уровни энергии) и $x = \frac{2}{3}\eta$ (которая вообще является локальным максимумом и не интересна), а также нетривиальная траектория - инстантон:

$$\frac{dx}{\sqrt{2U(x)}} = d\tau \Rightarrow x_{cl}(\tau) = \frac{\eta}{\cosh^2 \frac{\omega\tau}{2}}$$

Эта траектория - «отскок» («bounce trajectory»), на ней частица «скатывается» с локального максимума $x = 0$ вправо, закатывается на точку остановки $x = \eta$, а затем скатывается обратно и опять закатывается на $x = 0$. Сама траектория изображена на рисунке: Как обычно, центр инстантона может быть выбран произвольным: $x_{cl}\left(\tau - \tau_c\right), \tau_c \in (-\beta/2, \beta/2)$ – с чем, как обычно, будет связано наличие нулевой моды в этом функциональном интеграле. Действие на этом инстантоне считается тривиально, используя закон сохранения энергии:

$$S_0 = \int\limits_{-\infty}^{\infty} \left(\partial_\tau x_{cl}\right)^2 d\tau = 2\omega\eta^2 \int\limits_{-\infty}^{\infty} \frac{\sinh^2 z}{\cosh^6 z} dz = \frac{8}{15}\omega\eta^2 \gg 1$$

Квадратичные флуктуации Мы делаем разложение вблизи инстантона, и получаем $S_E\left[x_{cl}(\tau) + z(\tau)\right] \approx S_0 + S_2[z(\tau)]$ и

$$S_2[z(\tau)] \approx \frac{1}{2}\int z(\tau)\left(-\partial_\tau^2 + U''\left(x_{cl}(\tau)\right)\right) z(\tau) d\tau$$

Как обычно, мы имеем дело с оператором типа «уравнения Шрёдингера» $\hat{L} = -\partial_\tau^2 + U''\left(x_{cl}(\tau)\right)$. «отенциальная энергия» этого уравнения следующая:

$$U''\left(x_{cl}(\tau)\right) = \omega^2\left(1 - \frac{3}{\cosh^2 \frac{\omega\tau}{2}}\right)$$

Потенциал опять имеет вид Пешля-Теллеря $\left(\sim \frac{1}{\cosh^2 x}\right)$, поэтому для этой задачи опять можно найти аналитическое решение. Нам опять необходимо решать задачу поиска спектра оператора:

$$\hat{L}\psi_n(\tau) = \epsilon_n \psi_n(\tau)$$

У оператора имеется нулевая мода, связанная с произвольностью выбора центра инстантона, и она устроена аналогично:

$$\psi_1(\tau) = \frac{1}{\sqrt{S_0}} \frac{\partial x_{cl}}{\partial \tau}$$

Тут возникает третий важный момент, который отличается от рассматриваемого ранее двухъямного потенциала. Траектория $x_{cl}(\tau)$ имеет максимум, поэтому нулевая мода имеет узел. Она не может давать волновую функцию основного состояния - а только первого возбуждённого. Это означает, что основное состояние даёт отрицательную моду $\epsilon_0 = -|\epsilon_0| < 0$, и Гауссов интеграл по ней, устроенный как $\int dc_0 e^{\frac{1}{2}c_0^2|\epsilon_0|}$ - расходится! Тем не менее, давайте закроем глаза и на это, и воспользуемся стандартной формулой, говорящей, что этот интеграл равен $\sqrt{\frac{2\pi}{\epsilon_0}} = \pm i\sqrt{\frac{2\pi}{|\epsilon_0|}}$. Действительно, поскольку мы ожидаем наличие именно метастабильного состояния с комплексной энергией, мнимый вклад - это как раз то, что нам следует ожидать! (вещественный вклад означал бы лишь, что уровень энергии как-то изменился - и это не то, что нам интересно). Мистическим образом, поступая так, мы теряем двойку - и это четвёртый важный момент, который мы обсудим ниже.

Отщепляя интегрирование по нулевой моде, которое устроено точно так же и даёт $\sqrt{\frac{S_0}{2\pi}}\omega\beta$, и учитывая эту «потерянную» двойку, мы приходим к следующему ответу:

$$\frac{G_E(0,0,\beta)}{G_0(0,0,\beta)} = \pm ie^{-S_0}\frac{1}{2}\sqrt{\frac{S_0}{2\pi}}\omega\beta \cdot \left(-\frac{\det'\left(-\partial_\tau^2 + U''\left(x_{cl}(\tau)\right)\right)}{\det'\left(-\partial_\tau^2+\omega^2\right)}\right)^{-1/2}$$

Отношение определителей проще сосчитать, используя метод Гельфанда-Яглома; оно оказывается равным

$$\frac{\det'\left(-\partial_\tau^2 + U''\left(x_{cl}(\tau)\right)\right)}{\det'\left(-\partial_\tau^2+\omega^2\right)} = -\frac{1}{60}$$

(как и следовало ожидать, из-за отрицательной моды определитель тоже отрицателен). Наконец, суммирование разреженного инстантонного газа также тривиально - количество траекторий-отскоков может быть произвольным $n = 0, 1, ...$, и инстантонный газ даст попросту превратит найденное нами число (вклад с $n = 1$) в экспоненту от него же $\sum\limits_{n=0}^{\infty} \frac{1}{n!}\left(\pm i\Gamma_0\beta/2\right)^n = \exp\left(\pm i\Gamma_0\beta/2\right)$. Собирая всё вместе, мы получаем следующий ответ:

$$\frac{G_E(0,0,\beta)}{G_0(0,0,\beta)} = \exp\left(\pm ie^{-S_0}\frac{1}{2}\sqrt{\frac{30S_0}{\pi}}\omega\beta\right)$$

Сравнивая с ожидаемым ответом $\exp\left(i\Gamma_0\beta/2\right)$, мы понимаем, что необходимо выбрать знак «+» и ответ даётся:

$$\Gamma_0 = \omega\sqrt{\frac{30S_0}{\pi}}e^{-S_0} = \frac{4}{\sqrt{\pi}}\omega \cdot \sqrt{\omega\eta^2}e^{-8\omega\eta^2/15}$$

11.6.2

Обсуждение вопросов

Итак, к этому моменту у внимательного читателя могло накопиться порядочное количество вопросов, которые мы старались отмечать по ходу текста. Основной вопрос, конечно, можно сформулировать следующим образом: как мы берём расходящийся (sic!) вещественный интеграл, и получаем конечный и мнимый (sic!) ответ?!

Ответ кроется в процедуре аналитического продолжения. Исходный функциональный интеграл хорошо определён и является аналитической функцией на вещественной оси времени $t \in \mathbb{R}$. Мы строим его аналитическое продолжение в комплексную плоскость, и рассматриваем его на мнимой оси $t = -i\beta$. К сожалению, если буквально подставить мнимое время в функциональный интеграл, мы действительно получаем расходящийся интеграл - и это означает, что процедура такого аналитического продолжения устроена чуть сложнее; ниже мы обсудим, как именно.

С другой стороны, в мнимом времени инстантонная траектория - вещественная, что очень хорошо! Для взятия соответствующего интеграла мы можем пользоваться обычным вещественным методом перевала, для которого у нас имеется хорошо развитая интуиция. В терминах исходного интеграла - у него тоже, конечно, имеется седло, но оно комплексное - и значит, нам требуется комплексный метод перевала (для многомерного комплексного интеграла!). Более того, комплексных сёдел в действительности очень много, и задача определения тех, которые всё-таки дают вклад в интеграл нетривиальная задача [12]. Именно поэтому мы делаем Виковский поворот - он значительно упрощает нам жизнь. Цена, которую приходится заплатить за это упрощение — необходимость аналитического продолжения — в действительности невелика. Процедура аналитического продолжения (формально) Формально такую процедуру можно устроить следующим образом. Рассмотрим функциональный интеграл как аналитическую функцию трёх параметров λ, η, t. При этом (λ, η, t) соответствует исходному функциональному интегралу, а $(\lambda, \eta, -i\beta)$ - Евклидовому, который мы считаем. Проследим, как меняется действие при вращении $t = |t|e^{-i\varphi}$:

$$iS\left[x(\tau), \lambda, \eta, |t|e^{-i\varphi}\right] = \int\limits_{-\tau/2}^{\tau/2} d\tau \left(\frac{1}{2}e^{i\frac{\pi}{2}+i\varphi}\left(\partial_\tau x\right)^2 - e^{i\frac{\pi}{2}-i\varphi}\lambda x^2(\eta - x)\right)$$

При сопровождающем вращении $\lambda = |\lambda|e^{i\varphi}$ интеграл будет оставаться сходящимся (т.к траектории с большими $x(\tau)$ дают осциллирующий вклад), поэтому аналитическое продолжение $(\lambda, \eta, t) \to (|\lambda|e^{i\varphi}, \eta, |t|e^{-i\varphi})$ происходит тривиально, используя исходное выражение. При таком аналитическом продолжении при $\varphi = \frac{\pi}{2}$ мы получаем Евклидово действие (в мнимом времени), но с параматром $i\lambda : G_E(i\lambda, \eta, \beta)$. Нетривиальной остаётся процедура аналитического продолжения $\lambda \to -i\lambda$, потому что при буквально такой подстановке в интеграл он теряет свою сходимость. То, как устроено такое аналитическое продолжение, мы продемонстрируем на модельном (обычном) интеграле. Модельный интеграл Конечно, для функционального интеграла процедуру аналитического продолжения в явном виде предоставить достаточно тяжело - но ключевые её моменты (включая «мистическую двойку») можно ухватить на простом модельном одномерном интеграле. Рассмотрим следующий интеграл:

$$I(g) = \int\limits_{-\infty}^{\infty} dx \cdot \exp\left(-\frac{x^2}{2} + igx^3\right)$$

Полученная функция аналитична при $g \in \mathbb{R}$ (аналог «вещественного времени»). С другой стороны, если мы попытаемся «наивно» её продолжить в $g \to \mp ig$ (аналог нашего «мнимого времени»), мы немедленно получим расходящийся интеграл, который даже внешне похож на наш: $I(\pm ig) \simeq \int\limits_{-\infty}^{\infty} dx \exp\left(-\frac{x^2}{2} \pm gx^3\right)$. Тем не менее, процедуру аналитического продолжения можно построить достаточно просто. Заметим, что при комплексном $g = |g|e^{-i\varphi}$, интеграл сходится в комплексной плоскости в следующих

секторах комплексной плоскости:

$$\mathrm{Im}\left(gx^3\right) \geq 0 \leftrightarrow \begin{cases} \frac{\varphi}{3} & \leq \arg x \leq \frac{\pi}{3} + \frac{\varphi}{3} \\ \frac{2\pi}{3} + \frac{\varphi}{3} & \leq \arg x \leq \pi + \frac{\varphi}{3} \\ \frac{4\pi}{3} + \frac{\varphi}{3} & \leq \arg x \leq \frac{5\pi}{3} + \frac{\varphi}{3} \end{cases}$$

При $\varphi = 0$ наші интеграл $I(g)$ проходит по контуру, который лежит в первом секторе (вещественная ось). Поэтому если при уходе g в комплексную плоскость мы будем вращать соответствующим образом контур интеграла (чтобы он оставался в первой области), то полученный интеграл будет сходится, а также будет являться аналитической функцией g. Тем самым, аналитическое продолжения интеграла $I(g)$ строится следующим образом:

$$I(g) = \int\limits_C dx \exp\left(-\frac{x^2}{2} + igx^3\right), \quad C = \left\{\arg x \in \left[\frac{\varphi}{3}; \frac{\pi}{3} + \frac{\varphi}{3}\right]\right\}, \quad \varphi = -\arg g \in (-\pi, \pi)$$

(например, мы можем попросту вращать контур так, чтобы $\arg x = \frac{1}{3}\varphi$ - и интеграл всегда оставался осциллирующим). Теперь можно приступить к исследованию асимптотик полученной аналитической функции при $g \ll 1$, для чего можно применить метод перевала. У интеграла имеются две седловых точки:

$$\varphi(x) = -\frac{x^2}{2} + igx^3, \quad \varphi'(x) = -x + 3igx^2 \Rightarrow \begin{cases} x_1 = 0 \\ x_2 = \frac{-i}{3g} \end{cases}, \quad \varphi(x) = \begin{cases} 0, & x = x_1 \\ \frac{1}{54g^2}, & x = x_2 \end{cases}$$

$$\varphi''(x) = -1 + 6 \text{ igx } = \begin{cases} -1, & x = x_1 \\ 1, & x = x_2 \end{cases}$$

1. Первая седловая точка $x = x_1$ - тривиальная, она является аналогом нашего тривиального «осцилляторного» седла - траектории $x_{cl} = 0$. Она всегда вещественная, и вклад от неё не зависит от g. Направление наискорейшего спуска на ней соответствует действительной оси, и это седло всегда даёт вклад в интеграл. Сам вклад устроен следующим образом:

$$I_1(g) \approx \int\limits_{-\infty}^{\infty} e^{-x^2/2} dx = \sqrt{2\pi}$$

2. Вторая седловая точка - наш «инстантон». Для интеграла в «реальном времени» ($g \in \mathbb{R}$) она комплексна, и если бы мы не знали ничего о комплексных числах - мы бы её попросту упустили. Вторая производная в ней положительна - поэтому с точки зрения обычного Гауссового интегрирования, интеграл по ней расходился бы $\left(\sim \int\limits_{-\infty}^{\infty} dx e^{x^2}\right)$ - впрочем, мы знаем,что в действительности это означает, что направление наискорейшего спуска на ней идёт параллельно мнимой оси. С учётом этого, вклад от второго седла оказывается следующщй:

$$I_2(g) \approx \pm i\sqrt{2\pi} e^{1/54g^2}$$

В «мнимом времени» $g = \pm i|g|$ седло становится вещественным $x_2 = \mp\frac{1}{3|g|}$, а вклад от него - экспоненциально мал $\propto \exp\left(-1/54|g|^2\right)$, а также он чисто мнимый (хотя, напомним, подынтегральное выражение выглядит чисто вещественным $\int\limits_C e^{-x^2/2+gx^3} dx\Big)$. Так или иначе, аналогия тут практически полная. Для того, чтобы понять, как устроен вклад этой седловой точки, можно проследить устройство топологии комплексной плоскости

при вращении $g \to ge^{-i\pi/2}$(смотри рисунки). Какой вывод стоит сделать из рисунка? При $\varphi < \frac{\pi}{2}$, вклад приходит только от тривиального седла и интеграл оценивается как

$$I\left(|g|e^{-i\varphi}\right) \approx I_1(g) \approx \sqrt{2\pi}, \quad 0 \le \varphi < \frac{\pi}{2},$$

в то время как при $\varphi > \frac{\pi}{2}$, вклад даёт также и второе седло (причём направление наискорейшего спуска $+\frac{\pi}{2}$, поэтому знак $\operatorname{Im} I(g) > 0$) и оценка получается следующей:

$$I\left(|g|e^{-i\varphi}\right) \approx I_1(g) + I_2(g) \approx \sqrt{2\pi}\left(1 + ie^{1/54g^2}\right), \quad \pi > \varphi > \frac{\pi}{2}.$$

В действительности мы тут имеем дело с явлением Стокса. У функции $I(g)$ мнимая ось (а именно она нас интересует!) - это линия Стокса, на которой появляется экспоненциально малый вклад $e^{-1/54|g|^2}$ на фоне «большого» вклада от основного седла. Обычно это означает, что на самой линии Стокса экспоненциально малый вклад плохо определён - ведь с «большим» вкладом $I_1(g)$ связан асимптотический ряд, погрешность которого больше экспоненциально малого вклада $I_2(g)$. Однако в данном случае (как и в функциональном интеграле) экспоненциально малый вклад выделить всё-таки возможно, потому что только он - мнимый (в этом смысле в $\operatorname{Im} I(g)$ мы сравниваем не $|I_2(g)|$ с $|I_1(g)|$, а с нулём - такое сравнение вполне законно).

Что же происходит на самой линии Стокса? Глядя на рисунок мы видим, что мы должны деформировать контур таким образом, что мы проходим по вещественной оси через первое седло, доходим до второго (но вдоль линии наискорейшего возрастания!); а затем на втором седле начинаем двигаться вдоль линии наискорейшего спуска, которая параллельна мнимой оси - тем самым, второе седло строго на линии Стокса даёт половинный вклад $\frac{1}{2}I_2(g)$:

$$\operatorname{Im} I(-i|g|) \approx \frac{1}{2}I_2(g)$$

Выводы Наш модельный интеграл оказался крайне полезным. На нём мы поняли смысл отрицательной моды, и законность нашего способа работы с ней, ровно как и происхождение множителя $\frac{1}{2}$. В функциональном интеграле мы также имеем дело с явлением Стокса (как аналитической функции амплитуды потенциала, или, что эквивалентно, туннельного действия) - асимптотический ряд, связанный с ангармонизмом осциллятора ($\frac{\omega}{2}$ - это лишь нулевой порядок!) имеет экспоненциально малую погрешность, которая сравнима с шириной уровня Г. Последняя, тем не менее, хорошо определа, поскольку является чисто мнимой [13] (на самом деле, точно такое же явление Стокса происходит и в задаче о туннельном расщеплении). Дальнейшее аналитическое продолжение $(\lambda, \eta, -i\beta) \to (\lambda, \eta, t)$ в конечном итоге сохранит эту $\frac{1}{2}$, поскольку мы всё время остаёмся на линии Стокса по переменной λ; поэтому конечный ответ именно такой.

Метастабильные состояния Д Другой вопрос был связан с тем, как мы интерпретировали метастабильные состояния в частности, раскладывались по ним, как будто они образуют базис. Разложение, конечно, правильно проводить по всем состояниям непрерывного спектра. Тем не менее, квазистационарные состояния проявляют себя как полюса амплитуды рассеяния - S-матрицы - расположенные вблизи вещественной оси. При вычислении различных интегралов по непрерывному спектру (ну, например - функции Грина) именно эти состояния будут давать наибольший (полюсной) вклад. Поэтому, хоть разложение буквально не запишется в нужном виде, но в действительности с хорошей точностью [14] эта формула всё-таки работает:

$$G(0,0,t) \simeq \sum_n |\langle 0|n\rangle|^2 e^{-iE_n t - \Gamma_n t/2},$$

О диаграммах Фейнмана

Теория

(пока хз)

О дальнейших развитиях

(в ктп подробнее в разы будет)

24.2 Space

Обсудим подробно свойства пространства и их применения в квантовой механике.
(мб в другое место перенесу)

24.2.1 Rotation of Euclidean Space

(поместил сюда, потому что очень редко нужны эти штуки.)

классическая теория вращения пространства

О применениях методов вращения пространства (??????!!!)

(нахрена я вообще учил бы их!!!???? пока главный вопрос. вроде итак умеем из линала это делать)

постановка задачи

(Кузьмин)
“Были" в фиксированной системе координат (СК).
Теперь пусть две декартовы СК:
$-S$ -исходная, координаты x, y, z $-\tilde{S}$ -"другая", координаты $\tilde{x}, \tilde{y}, \tilde{z}$
Начала отсчёта совпадают; обе правые, т.е.
правый винт, расположенный вдоль оси Z, движется в положительном направлении оси Z при вращении в плоскости XY в направлении от X к Y.
Положение одной СК относительно другой: 3 орта $\times 3$ координаты $= 9$ чисел; но: $9-3($ условия ортогональнности ортов $)-3($ длина орта равна единице $)=3$
Популярные способы выбора 3-х чисел. а) теорема Эйлера: Произвольное перемещение твёрдого тела, имеющего неподвижную точку, можно осуществить посредством вращения вокруг некоторой оси. [цитата из Г.
Голдстейн, Классическая механика] $\vec{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ и угол поворота ω Вопрос: справедлива ли теорема Эйлера в 4-х мерном евклидовом про-ве? б) углы Эйлера (α, β, γ): β -угол между осями Z и $\tilde{Z}$ α -угол между линией пересечения плоскостей XY и $\tilde{X}\tilde{Y}$ и осью Y; γ - угол между линией пересечения плоскостей XY и $\tilde{X}\tilde{Y}$ и осью $\tilde{Y}$. Укажите область значений углов Эйлера α, β, γ.
Операции для перехода от S к $\tilde{S}$:

$R_Z(\alpha) -$ поворот вокруг оси Z на угол α
$R_{Y'}(\beta) -$ поворот вокруг оси Y' на угол β
$R_{Z'}(\gamma)$ - поворот вокруг оси Z' на угол γ

Пусть $|jm\rangle$ -вектор состояния "тела" с заданными значениями j и проекции на ось Z, $|\widehat{jm}\rangle$ - вектор состояния "тела" с заданными значениями j и проекции на ось $\tilde{Z}$. Перевод "тела" из одного состояния в другое

$$|\widehat{jm}\rangle = R(\omega)|jm\rangle$$

ω - параметры преобразования "тела".

оператор конечных вращений

Действие оператора поворота "тела" вокруг оси Z на угол α

$$R_Z(\alpha)f(r,\theta,\phi) = f(r,\theta,\phi-\alpha)$$

$R_Z(\alpha) = \exp\left(-\alpha\frac{d}{d\phi}\right), \ell_Z = \frac{\hbar}{i}\frac{d}{d\phi}, R_Z(\alpha) = \exp\left(-i\alpha\ell_Z\right)$, здесь и далее $\hbar = 1$

$$R(\omega) = \exp\left(-i\gamma\ell_{Z'}\right)\exp\left(-i\beta\ell_{Y'}\right)\exp\left(-i\alpha\ell_Z\right)$$

Повороты вокруг "подвижных" осей.

Как вычислять действие такого оператора на функции, заданные в "неподвижных" осях?

Перевод "тела" из одного состояния в другое

$$|\widehat{jm}\rangle = R(\alpha,\beta,\gamma)|jm\rangle$$

α,β,γ - параметры преобразования "тела"; сокращённое обозначение, ω.

Показали:

$$R(\omega) = \exp\left(-i\gamma\ell_{Z'}\right)\exp\left(-i\beta\ell_{Y'}\right)\exp\left(-i\alpha\ell_Z\right)$$

Повороты вокруг "подвижных" осей!

переход от подвижных осей к неподвижным

Связь поворота вокруг оси $\vec{a}$ на угол Φ с поворотом вокруг оси $\vec{b}$:

$$R_{\vec{a}}(\Phi) = R(\vec{b}\to\vec{a})R_{\vec{b}}(\Phi)R^{-1}(\vec{b}\to\vec{a})$$
$$R(\omega) = R_{Z'}(\gamma)R_{Y'}(\beta)R_Z(\alpha)$$
$$R_{Z'}(\gamma) = R_{Y'}(\beta)R_Z(\gamma)R^{-1}_{Y'}(\beta)$$
$$R_{Y'}(\beta) = R_Z(\alpha)R_Y(\beta)R^{-1}_Z(\alpha)$$
$$R(\omega) = R_Z(\alpha)R_Y(\beta)R^{-1}_Z(\alpha)\cdot R_Z(\gamma)\cdot R^{-1}_{Y'}(\beta)\times R_{Y'}(\beta)R_Z(\alpha) =$$
$$= R_Z(\alpha)R_Y(\beta)R^{-1}_Z(\alpha)\cdot R_Z(\gamma)\times R_Z(\alpha) =$$
$$= R_Z(\alpha)R_Y(\beta)R_Z(\gamma)$$
$$R(\alpha,\beta,\gamma) = \exp\left(-i\alpha\ell_Z\right)\exp\left(-i\beta\ell_Y\right)\exp\left(-i\gamma\ell_Z\right)$$

Все операторы относятся к исходному положению "тела".

матрицы конечных вращений

Поскольку $\ell^2 = \ell^2_X + \ell^2_Y + \ell^2_X,$ то $\left[\ell^2, R(\omega)\right]_- = 0,$ и $\ell^2|\widetilde{lm}\rangle = \ell^2 R(\omega)|lm\rangle = l(l+1)|\widetilde{lm}\rangle$

$$R(\omega)\psi_{lm} = \sum_{m_\prime} \psi_{lm'} \left(\psi_{lm'}, R_Z(\alpha)R_Y(\beta)R_Z(\gamma)\psi_{lm}\right) = \sum_{m_\prime} \mathcal{D}^l_{m'm}(\alpha,\beta,\gamma)\psi_{lm'}$$

Определим:

$$\mathcal{D}^l_{m'm}(\alpha,\beta,\gamma) \equiv \left(\psi_{lm'}, R_Z(\alpha)R_Y(\beta)R_Z(\gamma)\psi_{lm}\right)$$

тогда:

$$R_Z(\alpha) = \exp\left(-i\alpha\ell_Z\right),$$

$$\left(\psi_{lm'}R_Z(\alpha)\psi_{ln}\right) = \exp\left(-i\alpha m'\right)\delta\left(n-m'\right)$$

Поэтому запишем:

$$\begin{aligned}\mathcal{D}^l_{m'm}(\alpha,\beta,\gamma) &= \exp\left(-i\alpha m'\right)\exp(-i\gamma m)\left(\psi_{lm'}, R_Y(\beta)\psi_{lm}\right) = \\ &= \exp\left(-i\alpha m'\right)\exp(-i\gamma m)d^l_{m'm}(\beta)\end{aligned}$$

и определим

$$d^l_{m'm}(\beta) \equiv \left(\psi_{lm'}, \exp\left(-i\beta\ell_Y\right)\psi_{lm}\right)$$

пример: вращения со спином 1/2

$$s_{x,y,z} = \tfrac{\sigma_{x,y,z}}{2},\ \text{где}\ \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \sigma^2_{x,y,z} = I$$

$$s_z\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \tfrac{1}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad s_z\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\tfrac{1}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}, R_Z(\alpha)\psi_{1/2,\pm1/2} = \exp(\mp i\alpha/2)\psi_{1/2,\pm1/2}$$

$$\begin{aligned}R_Y(\beta) &= \exp\left(-i\beta\sigma_y/2\right) = \exp\left(-i\frac{\beta}{2}\sigma_y\right) = \cos\frac{\beta}{2}I - i\sin\frac{\beta}{2}\sigma_y = \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\cos\frac{\beta}{2} + \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\sin\frac{\beta}{2} = \begin{pmatrix} \cos\beta/2 & -\sin\beta/2 \\ \sin\beta/2 & \cos\beta/2 \end{pmatrix}\end{aligned}$$

(кривая таблица, потом переклею ее:)

$d^{1/2}_{m'm}(\beta):$	$-1/2$	$1/2$
$-1/2$	$\cos\beta/2$	$\sin\beta/2$
$1/2$	$-\sin\beta/2$	$\cos\beta/2$

$$R(\alpha,\beta,\gamma) = \exp\left(-i\alpha J_Z\right)\exp\left(-i\beta J_Y\right)\exp\left(-i\gamma J_Z\right)$$

Основные методы описания вращения

суть спина

(типичный вопрос, на который нужно ответить)

Методы вращения пространства в двух словах

(?? какие тут формулы?)
полный набор наблюдаемых составляют $\{s^2, s_z\}$.
(в строчку поясню, почему)
(далее методы вращения от рел квант мех)

Типичные примеры вращения пространства

(думаю, тут без ключевых примеров никуда не уйти.)

О применениях методов вращения пространства

(??? так где это нужно по итогу???)
(мб тут укажу, что в квантовых компьютерах, там вроде есть повороты кубитов??)

операторы поворота

(выпишу суть потом. пока не владею этой теорией)
(???? начало упущено)
ного умножения

$$\hat{R}(\alpha, \beta, \gamma) = \hat{R}_{z'}(\gamma) \cdot \hat{R}_{y'}(\beta) \cdot \hat{R}_z(\alpha)$$

где мы указали в качестве аргументов углы поворотов, а соответствующие оси вращений как нижние индексы.

Точный вид первого операторного фактора нам уже известен:

$$\hat{R}_z(\alpha) = e^{\mathrm{i}\hat{s}_z\alpha}, \quad \hat{s}_z = \frac{1}{2}\boldsymbol{\sigma}_3$$

Для определения второго фактора необходимо знать выражение для генератора $\hat{s}_{y'}$, запишем его в виде

$$\hat{s}_{y'} = \frac{1}{2}\left(\hat{\boldsymbol{\sigma}}' \cdot \boldsymbol{e}_{y'}\right)$$

где $e_{y'}$ -единичный вектор вдоль оси y', а $\hat{\sigma}'$ -матрицы Паули в базисе $\{x', y', z\}$.

Таким образом, это - оператор, который получается при вращении вокруг оси z на угол α и сходного оператора

$$\hat{s}_y = \frac{1}{2}\left(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{e}_y\right)$$

согласно закону преобразования операторов

$$\left(\hat{\boldsymbol{\sigma}}' \cdot \boldsymbol{e}_{y'}\right) = \hat{R}_z(\alpha) \cdot \left(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{e}_y\right) \cdot \hat{R}_z^\dagger(\alpha),$$

откуда сразу получаем

$$\hat{R}_{y'}(\beta) = \hat{R}_z(\alpha) \cdot \hat{R}_y(\beta) \cdot \hat{R}_z^\dagger(\alpha)$$

так что

$$\hat{R}_{z'}(\gamma) = \hat{R}_{y'}(\beta) \cdot \hat{R}_z(\gamma) \cdot \hat{R}_{y'}^\dagger(\beta)$$

значит

$$\hat{R}(\alpha, \beta, \gamma) = \hat{R}_{z'}(\gamma) \cdot \hat{R}_{y'}(\beta) \cdot \hat{R}_z(\alpha) = \hat{R}_{y'}(\beta) \cdot \hat{R}_z(\gamma) \cdot \hat{R}_{y'}^\dagger(\beta) \cdot \hat{R}_{y'}(\beta) \cdot \hat{R}_z(\alpha)$$

Унитарность оператора вращений дает

$$\hat{R}^{\dagger}_{y'}(\beta)\cdot\hat{R}_{y'}(\beta)=\mathbb{1}$$

так что

$$\hat{R}(\alpha,\beta,\gamma)=\hat{R}_{y'}(\beta)\cdot\hat{R}_z(\gamma)\cdot\hat{R}_z(\alpha)=\hat{R}_z(\alpha)\cdot\hat{R}_y(\beta)\cdot\hat{R}^{\dagger}_z(\alpha)\cdot\hat{R}_z(\gamma)\cdot\hat{R}_z(\alpha)$$

$$\hat{R}^{\dagger}_z(\alpha)\cdot\hat{R}_z(\gamma)\cdot\hat{R}_z(\alpha)=\hat{R}_z(\gamma)$$

так как вращение на угол α компенсируется обратным вращением.

Окончательно находим

$$\hat{R}(\alpha,\beta,\gamma)=\hat{R}_z(\alpha)\cdot\hat{R}_y(\beta)\cdot\hat{R}_z(\gamma)$$

откуда сразу полу чаем

$$\hat{R}_{y'}(\beta)=\hat{R}_z(\alpha)\cdot\hat{R}_y(\beta)\cdot\hat{R}^{\dagger}_z(\alpha)$$

так что

$$\hat{R}_{z'}(\gamma)=\hat{R}_{y'}(\beta)\cdot\hat{R}_z(\gamma)\cdot\hat{R}^{\dagger}_{y'}(\beta)$$

значит

$$\hat{R}(\alpha,\beta,\gamma)=\hat{R}_{z'}(\gamma)\cdot\hat{R}_{y'}(\beta)\cdot\hat{R}_z(\alpha)=\hat{R}_{y'}(\beta)\cdot\hat{R}_z(\gamma)\cdot\hat{R}^{\dagger}_{y'}(\beta)\cdot\hat{R}_{y'}(\beta)\cdot\hat{R}_z(\alpha)$$

Унитарность оператора вращений дает

$$\hat{R}^{\dagger}_{y'}(\beta)\cdot\hat{R}_{y'}(\beta)=\mathbb{1}$$

так что

$$\hat{R}(\alpha,\beta,\gamma)=\hat{R}_{y'}(\beta)\cdot\hat{R}_z(\gamma)\cdot\hat{R}_z(\alpha)=\hat{R}_z(\alpha)\cdot\hat{R}_y(\beta)\cdot\hat{R}^{\dagger}_z(\alpha)\cdot\hat{R}_z(\gamma)\cdot\hat{R}_z(\alpha)$$

$$\hat{R}^{\dagger}_z(\alpha)\cdot\hat{R}_z(\gamma)\cdot\hat{R}_z(\alpha)=\hat{R}_z(\gamma)$$

так как вращение на угол α компенсируется обратным вращением.

Окончательно находим

$$\hat{R}(\alpha,\beta,\gamma)=\hat{R}_z(\alpha)\cdot\hat{R}_y(\beta)\cdot\hat{R}_z(\gamma)$$

Очевидно, что вывод этого выражения нигде не опирался на свойства операторов спина $\frac{1}{2}$ так что полученная формула справедлива для частиц произвольного спина.

В этом выражении все факторы строго определены.

Например, спинорный оператор конечных вращений получается последовательным перемножением матриц

$$\hat{R}_z(\alpha)=\cos\frac{\alpha}{2}+\mathrm{i}\boldsymbol{\sigma}_3\sin\frac{\alpha}{2}=\begin{pmatrix}\cos\frac{\alpha}{2}+\mathrm{i}\sin\frac{\alpha}{2} & 0\\ 0 & \cos\frac{\alpha}{2}-\mathrm{i}\sin\frac{\alpha}{2}\end{pmatrix}=\begin{pmatrix}e^{\mathrm{i}\alpha/2} & 0\\ 0 & e^{-\mathrm{i}\alpha/2}\end{pmatrix}$$

$$\hat{R}_y(\alpha)=\cos\frac{\beta}{2}+\mathrm{i}\boldsymbol{\sigma}_2\sin\frac{\beta}{2}=\begin{pmatrix}\cos\frac{\beta}{2} & \sin\frac{\beta}{2}\\ -\sin\frac{\beta}{2} & \cos\frac{\beta}{2}\end{pmatrix}$$

$$\hat{R}_z(\gamma)=\begin{pmatrix}e^{\mathrm{i}\gamma/2} & 0\\ 0 & e^{-\mathrm{i}\gamma/2}\end{pmatrix}$$

В явном виде умножение матриц дает

$$\hat{R}_S(\alpha,\beta,\gamma)=\begin{pmatrix}\cos\frac{\beta}{2}\cdot e^{\mathrm{i}(\gamma+\alpha)/2} & \sin\frac{\beta}{2}\cdot e^{\mathrm{i}(\alpha-\gamma)/2}\\ -\sin\frac{\beta}{2}\cdot e^{\mathrm{i}(\gamma-\alpha)/2} & \cos\frac{\beta}{2}\cdot e^{-\mathrm{i}(\gamma+\alpha)/2}\end{pmatrix}$$

Поэтому преобразование спинора запишется в виде

$$\psi_a^R(\boldsymbol{r}) = \left\{\hat{R}_S(\alpha,\beta,\gamma)\right\}_a^b \psi_b\left(\mathcal{R}^{\mathrm{T}}\boldsymbol{r}\right),$$

где мы записали спинорный оператор вращений в матричной форме и использовали латинские спинорные индексы, чтобы не возникло путаницы с греческими обозначениями углов Эйлера.

Здесь матрица вращений в координатном пространстве

$$\mathcal{R}^{\mathrm{T}} = \mathcal{R}^{\mathrm{T}}(\alpha,\beta,\gamma) = \mathcal{R}_z^{\mathrm{T}}(\alpha)\mathcal{R}_{y'}^{\mathrm{T}}(\beta)\mathcal{R}_{z'}^{\mathrm{T}}(\gamma)$$

определяется теми же углами Эйлера.

При этом пространственная часть оператора вращения дает

$$\hat{R}_r(\alpha,\beta,\gamma)\psi_b(\boldsymbol{r}) = \psi_b(\mathcal{R}\boldsymbol{r})$$

где

$$\hat{R}_r(\alpha,\beta,\gamma) = \hat{R}_z^r(\alpha)\cdot\hat{R}_y^r(\beta)\cdot\hat{R}_z^r(\gamma)$$

Определяются операторами орбитального момента.

В итоге, преобразование спинора предСтавляется в факторизованной форме как произведение зав исяших от углов Эйлера спинорного и орбитального операторов

$$\psi^R(\boldsymbol{r}) = \hat{R}_S\cdot\hat{R}^r\psi(\boldsymbol{r}), \quad \hat{R} = \hat{R}(\alpha,\beta,\gamma) = \hat{R}_S\cdot\hat{R}^r$$

Действ ие пространственных и спинорных операторов можно продемонстрировать слеДующим образом: рассм отрим оператор

$$\boldsymbol{\sigma}\cdot\boldsymbol{n}$$

где $\boldsymbol{\sigma}$ -матрицы Паули, а вектор $\boldsymbol{n}$ - единичный вектор вдоль радиус-вектора $\boldsymbol{r}$. Вектор определяющий ось z:

$$\boldsymbol{n} = \hat{R}^r\boldsymbol{e}_z\left(\hat{R}^r\right)^\dagger$$

где вращение производится, как мы видели, на углы Эйлера в обратном порядке: сначала вокруг оси z на угол γ, потом на угол β и затем лишь вокруг оси самого вектора $\boldsymbol{n}$ на угол α, так что координаты вектора $\boldsymbol{n}$ в исходной системе -

$$\boldsymbol{n} = \{\cos\gamma\cos\beta, \sin\gamma\cos\beta, \sin\beta\}$$

при этом, конечно, значение угла α никак ни сказывается на координатах вектора $\boldsymbol{n}$, так как он задает вращен ие вектора $\boldsymbol{n}$ вокруг его собственной оси.

Найдем собственные векторы

$$(\boldsymbol{\sigma}\cdot\boldsymbol{n})\chi_{(k)} = \lambda_k\chi_{(k)}$$

где нет суммирован ия по k, который задает номер собствен ного значения спинора χ^a с индексом $a = \{1,2\}$. Подействуем на предыдущее уравнен ие спинорным оператором вращений R_S и учтем его унитарность,

$$\hat{R}_S(\boldsymbol{\sigma}\cdot\boldsymbol{n})\hat{R}_S^\dagger\hat{R}_S\chi_{(k)} = \lambda_k\hat{R}_S\chi_{(k)}$$

$$\hat{R}_S(\boldsymbol{\sigma}\cdot\boldsymbol{n})\hat{R}_S^\dagger = \hat{R}_S\hat{R}^r\left(\boldsymbol{\sigma}\cdot\boldsymbol{e}_z\right)\hat{R}_S^\dagger\left(\hat{R}^r\right)^\dagger = \boldsymbol{\sigma}_{z'}\cdot\boldsymbol{e}_{z'}$$

$$\boldsymbol{\sigma}_{z'} \cdot \boldsymbol{e}_{z'} \psi_{(k)} = \lambda_k \psi_{(k)}$$

Значит, спиноры $\psi_{(k)} = \hat{R}_S \chi(k)$ удовлетворяют уравнению на собственные значения

$$\boldsymbol{\sigma}_{z'} \cdot \boldsymbol{e}_{z'} \psi_{(k)} = \lambda_k \psi_{(k)}$$

екции спина на заданную ось.

Поэтому в базисе собственных векторов

$$\boldsymbol{\sigma}_{z'} \cdot \boldsymbol{e}_{z'} = \boldsymbol{\sigma}_3$$

n

$$\boldsymbol{\sigma}_3 \psi_{1,2} = \pm \psi_{1,2}$$

'T.e.

$$\psi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \psi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\chi_{1,2} = \hat{R}_S^\dagger \psi_{1,2}$$

Tak ч'TO

$$\chi_1 = \begin{pmatrix} \cos\frac{\beta}{2} \cdot e^{-\mathrm{i}(\alpha+\gamma)/2} \\ \sin\frac{\beta}{2} \cdot e^{-\mathrm{i}(\alpha-\gamma)/2} \end{pmatrix}, \quad \chi_2 = \begin{pmatrix} -\sin\frac{\beta}{2} \cdot e^{\mathrm{i}(\alpha-\gamma)/2} \\ \cos\frac{\beta}{2} \cdot e^{\mathrm{i}(\gamma+\alpha)/2} \end{pmatrix}$$

на угол α приводит к введен ию общей фазы у этих собственн ых векторов.

О вращениях по Вигнеру (???)

(там его Д-функция и все такое, никак не усвоил, но по идее сюда могу суть этого подхода записать. начну с другого раздела вдали.)

Квантование нерелятивистского спина в двух словах

(??? зачем мы делаем то, что ниже??? вроде тут крутая теория, ее только потренировать нужно, и можно будет пользоваться. хотя, перенесу только в следующую часть потом)

Пусть s - эрмитовы матрицы, которые удовлетворяют коммутационным соотношениям генераторов группы вращений:

$$[s_\alpha, s_\beta] = \mathrm{i}\epsilon_{\alpha\beta\gamma} s_\gamma$$

Поэтому в полный набор наблюдаемых можно включить лишь один из генераторов, например, s_z, ведь два других генератора не коммутируют с ним и не могут иметь совместного с ним базиса собственных векторов.

Нулевой коммутатор у генератора вращений может быть только с самим собой или со скалярной величиной, которая не преобразуется при вращениях, поскольку собственное значение скалярной величины до вращения и после вращения не изменяется.

Из генераторов группы вращений можно построить лишь один независимый скаляр s^2.

Вычислим коммутатор

$$\left[s^2, s_\alpha\right] = [s_\beta s_\beta, s_\alpha]$$

с помощью тождества $[AB, C] = A[B, C] + [A, C]B$ откуда

$$[s_\beta s_\beta, s_\alpha] = s_\beta \left[s_\beta, s_\alpha\right] + \left[s_\beta, s_\alpha\right] s_\beta = i\epsilon_{\beta\alpha\gamma} \left(s_\beta s_\gamma + s_\gamma s_\beta\right)$$

Здесь в круглых скобках - симметричный относительно перестановок индексов β и γ тензор второго ранга - сворачивается с тензором $\epsilon_{\beta\alpha\gamma}$, антисимметричным по перестановкам тех же индексов β и γ, поэтому

$$\left[s^2, s_\alpha\right] = 0$$

и полный набор наблюдаемых составляют $\{s^2, s_z\}$.

Базис тензорных полей удовлетворяет уравнениям на собственные значения полного набора наблюдаемых для группы вращений:

$$\begin{aligned} s^2 \left|\lambda_s, m_s\right\rangle =& \lambda_s \left|\lambda_s, m_s\right\rangle, \\ s_z \left|\lambda_s, m_s\right\rangle =& m_s \left|\lambda_s, m_s\right\rangle \end{aligned}$$

Будем считать этот базис ортонормированным.

В силу (??) повышающий и понижающий генераторы $s_\pm = s_x \pm \mathrm{i} s_y$ коммутируют с квадратом спина:

$$\left[s^2, s_\pm\right] = 0$$

и это означает, что значение λ_s не меняется при действии бесконечно малых преобразований с генераторами $s_{x,y}$, но при действии тех же преобразований меняется значение m_s, так как в противном случае, эти генераторы коммутировали бы с s_z, что неверно.

Такое положение указывает, что одному и тому же значению λ_s отвечают несколько значений m_s, т.е. имеет место вырождение спектра собственных значений λ_s по значениям m_s. Между прочим, мы установили общее условие вырожденности спектра эрмитовой матрицы A : если эрмитова матрица A коммутирует с эрмитовыми матрицами B и C, но сами матрицы B и C не коммутируют между собой, то спектр собственных значений матрицы A вырожден, например, по собственным значениям в совместном базисе с матрицей B

Найдем действие повышающего и понижающего генератора на совместный базис $\left|\lambda_s, m_s\right\rangle$. Для этого сначала вычислим коммутаторы

$$\left[s_\pm, s_z\right] = \left[s_x, s_z\right] \pm \mathrm{i}\left[s_y, s_z\right] = -\mathrm{i} s_y \pm \mathrm{i} i s_x = \mp s_\pm$$

Тогда

$$s_z s_\pm \left|\lambda_s, m_s\right\rangle = \left(s_\pm s_z \pm s_\pm\right) \left|\lambda_s, m_s\right\rangle = \left(m_s \pm 1\right) s_\pm \left|\lambda_s, m_s\right\rangle$$

Значит, вектор $s_\pm \left|\lambda_s, m_s\right\rangle$ имеет собственные значения s_z, равные $m_s \pm 1$:

$$s_\pm \left|\lambda_s, m_s\right\rangle = N_\pm\left(\lambda_s, m_s\right) \left|\lambda_s, m_s \pm 1\right\rangle \quad \rightarrow \quad \left(s_\pm \left|\lambda_s, m_s\right\rangle\right)^\dagger = \left\langle\lambda_s, m_s\right| s_\mp = N_\pm\left(\lambda_s, m_s\right) \left\langle\lambda_s, m_s\right|$$

где мы задали комплексную фазу собственного вектора $\left|\lambda_s, m_s\right\rangle$ так, чтобы нормировочный коэффициент был бы вещественным.

Найдем нормировочный коэффициент $N_\pm\left(\lambda_s, m_s\right)$. Для этого заметим, что

$$s^2 = s_x^2 + s_y^2 + s_z^2 = s_+ s_- + \mathrm{i}\left[s_x, s_y\right] + s_z^2 = s_+ s_- - s_z + s_z^2$$

и аналогично

$$s^2 = s_x^2 + s_y^2 + s_z^2 = s_- s_+ - \mathrm{i}\left[s_x, s_y\right] + s_z^2 = s_- s_+ + s_z + s_z^2$$

Тогда

$$\left\langle\lambda_s, m_s\right| s_\mp s_\pm \left|\lambda_s, m_s\right\rangle = \left(s_\pm \left|\lambda_s, m_s\right\rangle\right)^\dagger s_\pm \left|\lambda_s, m_s\right\rangle = N_\pm^2\left(\lambda_s, m_s\right)$$

Т.е.

$$N_\pm^2\left(\lambda_s, m_s\right) = \left\langle\lambda_s, m_s\right| s_\mp s_\pm \left|\lambda_s, m_s\right\rangle = \left\langle\lambda_s, m_s\right| \left(s^2 - s_z^2 \mp s_z\right) \left|\lambda_s, m_s\right\rangle = \lambda_s - m_s\left(m_s \pm 1\right)$$

Поскольку нормировка вектора не может быть отрицательной, $N_{\pm}^{2}\left(\lambda_{s}, m_{s}\right) \geqslant 0$. Это условие может быть выполнено, только если в цепочках многократного действия повышающего и понижающего операторов, во-первых, значения m_s не произвольны, а принимают такие значения, чтобы

$$m_{s}\left(m_{s} \pm 1\right) \leqslant \lambda_{s}$$

и во-вторых, должны существовать максимальное $m_{s}^{\max}$ и минимальное $m_{s}^{\min}$ значения, которые дают в точности нулевые Значения нормы вектора после повышения и понижения, соответственно, так как в противном случае повышение и понижение приводило бы к возникновению векторов с отрицательной нормой, что недопустимо, т.е.

$$m_{s}^{\max}\left(m_{s}^{\max}+1\right)=\lambda_{s}, \quad m_{s}^{\min}\left(m_{s}^{\min}-1\right)=\lambda_{s}$$

Вместе с тем, действуя многократно на вектор $\left|\lambda_{s}, m_{s}^{\max}\right\rangle$ понижаюпим оператором n раз, мы получим $m_{s}=m_{s}^{\max}-n$ и в конце концов вектор, в Точности равный $\left|\lambda_{s}, m_{s}^{\min}\right\rangle$, в силу существования минимально допустимого значения m_s, т.е. для некоторого неотрицательного целого значения n верно $m_{s}^{\min}=m_{s}^{\max}-n$. Тогда связь минимального и максимального значений проекции спина на ось zс собственным значением квадрата спина λ_s приводит к единственному решению в виде

$$\begin{gathered}
m_{s}^{\max}\left(m_{s}^{\max}+1\right)-m_{s}^{\min}\left(m_{s}^{\min}-1\right)=0, \\
m_{s}^{\max}\left(m_{s}^{\max}+1\right)-\left(m_{s}^{\max}-n\right)\left(m_{s}^{\max}-n-1\right)=0, \\
m_{s}^{\max}=\tfrac{n}{2}, \quad m_{s}^{\min}=-\tfrac{n}{2}
\end{gathered}$$

Максимальное значение проекции спина на ось z обозначают символом s, так что

$$s=\frac{n}{2}$$

т.е. допустимые значения проекции спина - это положительные полуцелые и целые значения.

Целые значения отвечают полям, которые называют тензорными, а полуцелые - спинорным полям.

Базис полей, таким образом, образуют совместные собственные векторы квадрата спина и его проекции на выбранную ось, так что изменяя обозначения путем подстановки $\lambda_{s}=s(s+1) \mapsto s$ запишем его в виде

$$\left|s, m_{s}\right\rangle, \quad m_{s} \in\{-s,-s+1, ..., s-1, s\}$$

Действие повышающей и понижающей матрицы спина на базисные вектора строго определено,

$$s_{\pm}\left|s, m_{s}\right\rangle=\sqrt{s(s+1)-m_{s}\left(m_{s} \pm 1\right)}\left|s, m_{s} \pm 1\right\rangle$$

В частном случае $s = 1$, Мы убедились, что соотношения (3.36) являются тождествами согласно проведенной нами процедуре прямого построения матриц спина и собственных векторов для матрицы s_z. Размерность пространства собственных векторов квадрата спина и его проекции на выбранную ось равна один старший вектор с максимальным значением проекции и n шагов от старшего вектора до младшего, т.е. вектора с минимальным значением проекции, а значит,

$$k=1+n=1+2 s$$

Это число компонент называют мультиплетностью неприводимого представления группы вращений для поля.

Неприводимым это представление называют потому, что при вращениях, а значит, при многократном действии генераторов спина, век'тор с заданной проекцией спина на ось z перемешивается со всеми другими векторами базиса с тем же значением квадрата спина, т.е. пространство собственных векторов с заданным квадратом спина не содержит в себе подпространств, вектора которых не смешивались бы друг с другом при действии группы вращений.

Для скаляра $s = 0$, и поле имеет одну единственную компоненту, поэтому скаляр называют синглетом и обозначают символом 1.

У вектора $s = 1$, и поле имеет три компоненты, это - триплет 3, у спинора $s = \frac{1}{2}$, и поле имеет две компоненты, это -дублет 2

Напомним, что построенный нами базис называют стандартным, он решает задачу классификации полей по базису собственных векторов генераторов спина.

О связи спина со статистикой (????)

(?? тут Киселев о чем угодно рассуждает, нужно переписать нормально. да и вообще, переставить в следующую часть, а суть выписать в новый параграф)

Рассмотрим два тождественных фермиона.

Их волновая функция -

$$\left\langle \boldsymbol{r}_1, \theta^{\alpha}_{(1)}, n_1; \boldsymbol{r}_2, \theta^{\beta}_{(2)}, n_2 | \Psi \right\rangle = \psi^{(n_1,n_2)}_{\alpha\beta} \left(\boldsymbol{r}_1, \boldsymbol{r}_2 \right)$$

где мы указали возможные многомерные квантовые числа (n_1, n_2), не связанные со спинорными характеристиками.

После поворота на угол 2π координаты первой частицы r_1 и ее

$$\psi^{(n_1,n_2)}_{\alpha\beta} \left(\boldsymbol{r}_1, \boldsymbol{r}_2 \right) \overset{\mathcal{R}_1(2\pi)}{\longrightarrow} \psi^{\mathcal{R}_1(n_1,n_2)}_{\alpha\beta} \left(\boldsymbol{r}_1, \boldsymbol{r}_2 \right) = -\psi_{\alpha\beta} \left(\boldsymbol{r}_1, \boldsymbol{r}_2 \right)$$

Подобное отличие в фазе волновой функции фермионов после вращения на угол 2π моделируют ситуацию, когда квантовые числа двух ферм ионов тождествен но совпадают:

$$\boldsymbol{r}_1 = \boldsymbol{r}_2 = \boldsymbol{r}, \quad \theta^{\alpha}_{(1)} = \theta^{\beta}_{(2)} = \theta^1, \quad n_1 = n_2 = n$$

т.е., другим и словами, поместим тождественные частицы с одним и тем же набором значений наблюдаемых величин в одну точку пространства.

В полной аналогии с выводом допустимых значений квантованного орбитального момента потребуем выполнение следующего принци па: если состояния каждой из двух тождественных частиц не отличи мы, то вращение одной из них на угол 2π не наблюдаемо, т.е. должно приводить к тождественному преобразованию состояния.

По сути, речь идет о вращении одной частицы относительно одной точке, то такое вращение не имеет физического смысла, т.е. не наблюдаемо.

Следовательно, исходная волновая функция

$$\psi^{(n,n)}_{11}(\boldsymbol{r}, \boldsymbol{r})$$

должна тождественно совпадать с волновой функцией после вращения координат одной из частиц на угол 2π :

$$\psi^{(n,n)}_{11} \left(\mathbf{r}, \mathbf{r}' \right) = -\psi^{(n,n)}_{11}(\mathbf{r}, \boldsymbol{r}) \equiv 0$$

что достигается только в случае равенства нулю волновой функции тождественных фер-

.

(??)

Этот принцип автоматически удовлетворяется, если волновую функцию тождественных

(????)

$$\psi_{\alpha\beta}^{A(n_1,n_2)}(\boldsymbol{r}_1,\boldsymbol{r}_2)=\frac{1}{\sqrt{2}}\left\{\psi_{\alpha\beta}^{(n_1,n_2)}(\boldsymbol{r}_1,\boldsymbol{r}_2)-\psi_{\beta\alpha}^{(n_2,n_1)}(\boldsymbol{r}_2,\boldsymbol{r}_1)\right\}$$

так как она обращается в нуль, если квантовые состояния фермионов тождественны

А атисимметризованная волновая функция двух фермионов являет собой пример общего принципа, возникающего в Квантовой механике с тождествен ными частицами.

В самом деле, физическая система из тождествен ных частиц не изменится, если поменять местами пару этих частиц.

В квантовой механике это утвержден ие означает, что состояние системы

$$|\Psi:\{Q_1,Q_2,...\}\rangle=\lambda\,|\Psi:\{Q_2,Q_1,...\}\rangle\,,\quad |\lambda|=1$$

где $\{Q_1,Q_2,...\}$ -полный набор наблюдаемых для частиц $\{1,2,...\}$.В этом уравнении мы требуем, чтобы при перестановке квантовых чисел первой и второй частиц вектор состояния остался прежним с точностью до фазового множителя (нормировка остается без изменения).

Если ввести оператор перестановок

$$\hat{\delta}_{1\leftrightarrow 2}\,|\Psi:\{Q_1,Q_2,...\}\rangle=|\Psi:\{Q_2,Q_1,...\}\rangle$$

то (9.28) есть ни что и ное, как уравнение на собствен ные значения для.

Двукратное применение перестановки возвращает систему к исходному состоянию:

$$\hat{\mathcal{S}}\hat{\mathcal{S}}=1$$

откуда немедлен но следует, что спектр собственных значений оператора перестановок тождественных частиц

$$\lambda^2=1\leftrightarrow\quad \lambda=\pm 1$$

Поскольку перестановки не изменяют никаких наблюдаемых характеристик системы тождественных частиц, оператор перестановок коммутирует со всеми наблюдаемыми

$$[\hat{\mathrm{S}},\hat{H}]=[\hat{\mathrm{S}},\hat{\boldsymbol{p}}]=[\hat{\mathrm{s}},\hat{\boldsymbol{j}}]=...=0$$

Числа двух тождественных частиц совпадают.

Как мы видели, это имеет место Для фермионов - частиц с полуцелым сп ином.

В этом случае

$$\lambda=e^{2\pi\mathrm{i}s},$$

где s -значение сп ина каждой из тождественных частиц.

Эта формула, полученная для полуцелых значений спина частиц, остается справедлива и для целых значений спина, Т.е. для бозонов, которые, таким образом, имеют симметризованные по перестановкам волновые функции.

Именно, в природе не наблюдаются псевдо-бозоны целого спина с антисимметричным и по перестановкам волновыми функциями.

Тем не менее, поля так их частиц используются Для вспомогательных целей в квантовой теории поля для наиболее наглядной форм ули ровк и некоторых прин ципов сим метрии.

Поля псевдо-бозонов называют "гостам и" (от ан глийского ghost, Что значит "дух") или просто "духами".

При этом, ОДн ако, полагаЮт, что число духов в начальном и конечном состоянии равно нулю, т.е.

В полный набор наблюдаемых включают число ДУхов, тождественно равн ое нулю.

Подчеркнем, что рассмотренная связь спина со стати стикой возникла благодаря пространственной вращательной симметрии для спиноров, т.е.

благодаря группе $SU(2)$. ОДнако это не знач ит, что присутствие какой-либо Другой си мметри и со спинорами в группе $SU(2)$ так же неми нуемо при ведет к антисимметризации волновых функций.

Например, в стандартную модель взаимодействий элементарн ых части ц включено скалярное, а следовательно, бозонное, поле со спином 0, которое является спинором по калибровочной группе $SU(2)$. Как мы показали, нали чие калибровочной группы симметрии отвечает сохранению заряда, который в данном случае - заряд частицы в слабом взаимодействии.

Эта калибровочная группа никак не связана с пространственными вращениям и, и поэтом у она не означает введения каких-либо дополнительных ограни чений на волновую функцию, связанных с сим метрией по перестановкам.

Такие группы, не связанные с вращениям и пространства, называются группами внутрен ней симметрии.

Генераторы таких групп, следовательно, Коммутируют с генераторами вращений и трансляций

Квантование релятивистского спина в двух словах

О спине 1/2

Обсудим самое основное о спине $1/2$.

(?? не в теории поля ли это??)

Типичный вывод матриц Паули

(?? а какой еще мог бы быть вывод??)

(?? этот раздел точно тут должен быть?)

Рассмотрим поле с полуцелым спином, $s = \frac{1}{2}$. В этом случае соответствующая спиновая матрица представляется в виде

$$s = \frac{1}{2}\sigma$$

где σ - матрицы Паули.

Найдем явный вид матриц Паули, используя общие выражения для действия матриц спина на базисные поля.

Базис спиновых состояний для краткости обозначений записывают как

$$\left|\frac{1}{2}, +\frac{1}{2}\right\rangle = |+\rangle, \quad \left|\frac{1}{2}, -\frac{1}{2}\right\rangle = |-\rangle$$

причем это - собственные векторы проекции спина

$$s_z|+\rangle = \frac{1}{2}|+\rangle, \quad s_z|-\rangle = -\frac{1}{2}|-\rangle$$

Следовательно, эта матрица в рассматриваемом базисе имеет диагональный вид

$$s_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Согласно (3.36) ненулевые матричные элементы повышающего и понижающего операторов

$$\langle + |s_+| - \rangle = \sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right) - (-1)\frac{1}{2}\left(-\frac{1}{2}+1\right)} = 1$$
$$\langle - |s_-| + \rangle = (\langle + |s_+| - \rangle)^\dagger = 1$$

откуда

$$s_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad s_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Тогда обратное преобразование $s_\pm \leftrightarrow s_{x,y}$ дает

$$s_x = \frac{1}{2}(s_+ + s_-) = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
$$s_y = \frac{1}{2\mathrm{i}}(s_+ - s_-) = \frac{1}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$$

Поэтому сигма-матрицы Паули - это

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

О спинах

О популярных аналогиях спина

(тут примеры, как про него думать можно и насколько корректно это? пока такое не готовил. например, там если я повращаюсь и изменю внутреннюю стрелку на противоположную. насколько так можно думать?)

Примеры спинов и спиноров

(самые частые тут укажу, чтобы конкретику тоже иметь)

О моделях из спинов

(их полным полно, укажу лишь самые типичные)

О том, как взаимодействуют разные спины, если они разные предствления (??)

(такой вопрос все еще есть, разве что мб это больше в теорию поля. пока связь ее с квантмехом не отработана.)

24.2.2 Wigner D-Function

Wigner D-Function

основные свойства D-функций Вигнера

1.

Унитарность $\overline{D}$ - комплексно-сопряжённая функция

$$\sum_{m=-j}^{j} \overline{\mathcal{D}}^{j}_{m,n}(\alpha,\beta,\gamma)\mathcal{D}^{j}_{m,n'}(\alpha,\beta,\gamma) = \delta\left(n'-n\right)$$

2.

Ортогональность

$$\int_0^{2\pi}\int_0^{2\pi}\int_0^{\pi} \overline{\mathcal{D}}^{j}_{m,n}(\alpha,\beta,\gamma)\mathcal{D}^{j'}_{m',n'}(\alpha,\beta,\gamma)\sin\beta d\beta d\gamma d\alpha = \\ = \frac{8\pi^2}{2j+1}\delta\left(j'-j\right)\delta\left(m'-m\right)\delta\left(n'-n\right)$$

Свойства $\mathcal{D}$ -функций

1.

Унитарность ($\overline{D--}\mathcal{D}$ -функция)

$$\sum_{m=-j}^{j} \overline{\mathcal{D}}^{j}_{m,n}(\alpha,\beta,\gamma)\mathcal{D}^{j}_{m,n'}(\alpha,\beta,\gamma) = \delta\left(n'-n\right)$$

2.

Ортогональность

$$\int_0^{2\pi}\int_0^{2\pi}\int_0^{\pi} \overline{\mathcal{D}}^{j}_{m,n}(\alpha,\beta,\gamma)\mathcal{D}^{j'}_{m',n'}(\alpha,\beta,\gamma)\sin\beta d\beta d\gamma d\alpha = \\ = \frac{8\pi^2}{2j+1}\delta\left(j'-j\right)\delta\left(m'-m\right)\delta\left(n'-n\right)$$

3.

Произведение двух D-функций одинаковых аргументов (см. домашнее задание лекции 5, слайд 5).

4.

Используя пункты 1 и 3, вычислите

$$\iiint \overline{\mathcal{D}}^{j}_{m,n}(\alpha,\beta,\gamma)\mathcal{D}^{j_1}_{m_1,n_1}(\alpha,\beta,\gamma)\mathcal{D}^{j_2}_{m_2,n_2}(\alpha,\beta,\gamma)\sin\beta d\beta d\gamma d\alpha$$

вычисление $D-$функции Вигнера

Вариант 1:

$$\mathcal{D}^{J}_{M'M}(\omega) = (\psi_{LM'}, R(\omega)\psi_{LM})$$

Вариант 2:

$$\mathcal{D}^{J}_{M'M}(\omega) = \sum_{m_1,m_2}\sum_{n_1,n_2}\langle j_1 m_1 j_2 m_2|JM\rangle\langle j_1 n_1 j_2 n_2|JM'\rangle\,\mathcal{D}^{j_1}_{n_1 m_1}(\omega)\mathcal{D}^{j_2}_{n_2 m_2}(\omega)$$

Вариант 3: Унитарное преобразование двух комплексных переменных z_1, z_2

$$z_1' = a_{11}z_1 + a_{12}z_2$$
$$z_2' = a_{11}z_1 + a_{12}z_2$$
$$\sum_k a_{ik}a^*_{jk} = \sum_k a_{ki}a^*_{kj} = \delta(j-i)$$

матрицы и векторы

$$Z=\begin{pmatrix} z_1 \\ z_2 \end{pmatrix}, Z'=WZ, W=\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, W^{\dagger}=\begin{pmatrix} a_{11}^{*} & a_{21}^{*} \\ a_{12}^{*} & a_{22}^{*} \end{pmatrix}$$

8 вещественных чисел.

Условие

$$W^{\dagger}W=\begin{pmatrix} a_{11}^{*}a_{11}+a_{21}^{*}a_{21} & a_{11}^{*}a_{12}+a_{21}^{*}a_{22} \\ a_{12}^{*}a_{11}+a_{22}^{*}a_{21} & a_{12}^{*}a_{12}+a_{22}^{*}a_{22} \end{pmatrix}=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}=I; \quad \text{4 уравнения}$$

Потребуем $\det W=1$. Унитарность даёт, $|\det W|=1$. 3 независимых вещественных параметра

$$W=\begin{pmatrix} a & b \\ -b^{*} & a^{*} \end{pmatrix}, \det W=|a|^2+|b|^2; \begin{array}{l} a=\exp(i\xi)\cos\omega \\ b=\exp(i\eta)\sin\omega \end{array}$$

Рассмотрим радиус-вектор с координатами (x,y,z) и построим эрмитову матрицу

$$\alpha=\begin{pmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{pmatrix}=\gamma I+x\sigma_x+y\sigma_y+z\sigma_z=\begin{pmatrix} \gamma+z & x-iy \\ x+iy & \gamma-z \end{pmatrix}$$

Матрица α эрмитова: $\alpha_{11}^{*}=\alpha_{11}, \alpha_{22}^{*}=\alpha_{22}, \alpha_{12}^{*}=\alpha_{21}, \alpha_{21}^{*}=\alpha_{12}$.

$$\gamma=\frac{1}{2}\left(\alpha_{11}+\alpha_{22}\right), x=\frac{1}{2}\left(\alpha_{12}+\alpha_{21}\right), y=\frac{1}{2i}\left(\alpha_{21}-\alpha_{12}\right), z=\frac{1}{2}\left(\alpha_{11}-\alpha_{21}\right)$$

преобразование матрицы α

$$\begin{gathered} \alpha\to\alpha'=W\alpha W^{\dagger}=\gamma' I+x'\sigma_x+y'\sigma_y+z'\sigma_z \\ \operatorname{Sp}(\alpha')=\operatorname{Sp}\left(W\alpha W^{\dagger}\right)=\operatorname{Sp}\left(W^{\dagger}W\alpha\right)=\operatorname{Sp}(\alpha)\to\gamma'=\gamma \\ \det\alpha'=\det\left(W\alpha W^{\dagger}\right)=\det\alpha\to\gamma'^2-\left(x'^2+y'^2+z'^2\right)=\gamma^2-\left(x^2+y^2+z^2\right) \\ x'^2+y'^2+z'^2=x^2+y^2+z^2 \end{gathered}$$

Если взять $W: W^{\dagger}W\neq I, \det W=1$, и $\gamma=ct$

$$\begin{gathered} (ct')^2-\left(x'^2+y'^2+z'^2\right)=(ct)^2-\left(x^2+y^2+z^2\right) \\ \alpha'=\begin{pmatrix} \gamma+\left(a^{*}b+ab^{*}\right)x+i\left(a^{*}b-ab^{*}\right)y+\left(|a|^2-|b|^2\right)z \\ \left(a^{*2}-b^{*2}\right)x+i\left(a^{*2}+b^{*2}\right)y-2a^{*}b^{*}z \\ \left(a^2-b^2\right)x-i\left(a^2+b^2\right)y-2abz \\ \gamma-\left(a^{*}b+ab^{*}\right)x-i\left(a^{*}b-ab^{*}\right)y-\left(|a|^2-|b|^2\right)z \end{pmatrix} \end{gathered}$$

Преобразование радиус-вектора

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}=\begin{pmatrix} \frac{1}{2}\left(a^2+a^{*2}-b^2-b^{*2}\right) & \frac{i}{2}\left(a^{*2}-a^2+b^{*2}-b^2\right) & -ab-a^{*}b^{*} \\ \frac{i}{2}\left(a^{*2}-a^2+b^{*2}-b^2\right) & \frac{1}{2}\left(a^2+a^{*2}+b^2+b^{*2}\right) & i\left(a^{*}b^{*}-ab\right) \\ \left(a^{*}b+ab^{*}\right) & i\left(a^{*}b-ab^{*}\right) & \left(|a|^2-|b|^2\right) \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Проверьте и подставьте выражения a и b через ξ,η и ω.

Выразите переменные ξ,η и ω через углы Эйлера.

$$\begin{gathered} \vec{x}'=M\vec{x}, \quad x'^2+y'^2+z'^2=x^2+y^2+z^2 \\ \gamma I+x'\sigma_x+y'\sigma_y+z'\sigma_z=\gamma I+W\left(x\sigma_x+y\sigma_y+z\sigma_z\right)W^{\dagger} \end{gathered}$$

Умножим обе части равенства слева на σ_l и возьмём шпур

$$x'_l = \frac{1}{2}\,\mathrm{Sp}\left(\sigma_l W\left(x\sigma_x + y\sigma_y + z\sigma_z\right)W^\dagger\right)$$

$$M_{lk} = \frac{1}{2}\,\mathrm{Sp}\left(\sigma_l W \sigma_k W^\dagger\right)$$

наблюдения от Кузьмина

(пока что я хз, к чему он вообще это дал)
Наблюдения
1.
Каждой унитарной матрице W соответствует ортогональная матрица M, причём единичной W соответствует единичная M.
2.
Пусть $W_1 \to M_1$ и $W_2 \to M_2$.

$$\alpha = \gamma I + \vec{x}\cdot\vec{\sigma};\quad \alpha \to \alpha' = W_1\alpha W_1^\dagger = \gamma I + \vec{x}_1\cdot\vec{\sigma};\quad \vec{x}_1 = M_1\vec{x}$$
$$\alpha' \to \alpha'' = W_2\alpha' W_2^\dagger = W_2W_1\alpha W_1^\dagger W_2^\dagger = (W_2W_1)\,\alpha\,(W_2W_1)^\dagger$$
$$\alpha'' = W_2\left(\gamma I + \vec{x}_1\cdot\vec{\sigma}\right)W_2^\dagger = \gamma I + \vec{x}_2\cdot\vec{\sigma},\quad \vec{x}_2 = M_2\vec{x}_1 = (M_2M_1)\,\vec{x}$$

Произведению матриц W_2W_1 соответствует произведение M_2M_1. 3.
При одновременной смене знаков у матричных элементов a и b матрица $W \to -W$, но $M \to M$. В частности, $W = \pm I$ отвечает единичная матрица $M = I$.

вкратце итог

Основная задача

$$R(\alpha,\beta,\gamma) = \exp\left(-i\alpha J_Z\right)\exp\left(-i\beta J_Y\right)\exp\left(-i\gamma J_Z\right)$$
$$R(\alpha,\beta,\gamma)\psi_{jm} = \sum_{n=-j}^{j}\psi_{jn}\left(\psi_{jn}, R_Z(\alpha)R_Y(\beta)R_Z(\gamma)\psi_{jm}\right) = \sum_{n=-j}^{j}\mathcal{D}^j_{n,m}(\alpha,\beta,\gamma)\psi_{jn}$$

Вспомогательная задача

$$\vec{x} = (x_1,x_2,x_3) \longleftrightarrow \alpha = \gamma I + \vec{x}\cdot\vec{\sigma},\quad \alpha^\dagger = \alpha;$$

$$W^\dagger = W, \det W = 1,\quad W = \begin{pmatrix} \exp(i\xi)\cos\omega & \exp(i\eta)\sin\omega \\ -\exp(-i\eta)\sin\omega & \exp(-i\xi)\cos\omega \end{pmatrix}$$
$$\alpha \to \alpha' = W\alpha W^\dagger \to \vec{x}'$$
$$x_1'^2 + x_2'^2 + x_3'^2 = x_1^2 + x_2^2 + x_3^2, x'_k = M_{kl}x_l,\quad M_{kl} = \mathrm{Sp}\left(\sigma_k W \sigma_l W^\dagger\right)$$
$$\text{Если } W_1 \to M_1, W_2 \to M_2, \text{ то } W_2W_1 \to M_2M_1$$
$$\text{Если } W \to M, \text{ то } (-W) \to M$$
$$\text{Если } W = \pm I, \text{ то } M[W] = I$$

Из домашнего задания

$$W(\omega = 0) \to M = \begin{pmatrix} \cos 2\xi & \sin 2\xi & 0 \\ -\sin 2\xi & \cos 2\xi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$W(\xi = \eta = 0) \to M = \begin{pmatrix} \cos 2\omega & 0 & -\sin 2\omega \\ 0 & 1 & 0 \\ \sin 2\omega & 0 & \cos 2\omega \end{pmatrix}$$

Идея: найти совокупность из $2j+1(j=0,1/2,1,...)$ линейно-независимых функций $B_{jm}(z_1,z_2),(m=-j,-j+1,...,j-1,j)$, таких, что

$$B_{jm}(z_1',z_2')=\sum_{m'=-j}^{j}A^j_{m',m}B_{jm'}(z_1,z_2),\text{ если }\begin{pmatrix}z_1'\\z_2'\end{pmatrix}=W\begin{pmatrix}z_1\\z_2\end{pmatrix}$$
$$A^j=A^j(W),\text{ и }A^{j\dagger}A^j=I$$
$$\text{Для } j=0, A^0=I, B_{00}=\text{const}$$
$$\text{для } j=1/2, A^{1/2}=W, B_{1/2,-1/2}=z_2, B_{1/2,1/2}=z_1$$

конечные вращения 2

внутренние квантовые числа

“Внутренние" квантовые числа

$$W=\begin{pmatrix}1+i\xi_3 & i\xi_1+\xi_2\\ i\xi_1-\xi_2 & 1-i\xi_3\end{pmatrix}=I+\delta W$$
$$\delta W=i\left[\begin{pmatrix}0&1\\1&0\end{pmatrix}\xi_1+\begin{pmatrix}0&-i\\i&0\end{pmatrix}\xi_2+\begin{pmatrix}1&0\\0&-1\end{pmatrix}\xi_3\right]=i\sum_{k=1}^{3}\tau_k\xi_k$$
$$t_k\equiv\tfrac{1}{2}\tau_k:[t_1,t_2]_-=it_3;\quad t_1^2+t_2^2+t_3^2=\tfrac{3}{4}=t(t+1)\to t=\tfrac{1}{2}$$

Пусть имеется s нуклонов.

Состояние будет задано числами $A_1,A_2,...A_s,A_j=1,2$ Временно забудем про статистику Ферми-Дирака, $\psi=\psi(A_1)\psi(A_2)...\psi(A_s)$.

$$\psi\to\phi=(W)_1(W)_2...(W)_s\psi_{A_1,A_2,...,A_s}$$

Для бесконечно-малых преобразований

$$\delta\psi=\sum_{j=1}^{s}(\delta W)_j\psi=\sum_{j=1}^{s}i\sum_{k=1}^{3}(\tau_k)_j\xi_k\psi=i\sum_{k=1}^{3}\xi_k\left[\sum_{j=1}^{s}(\tau_k)_j\right]\psi=i2\sum_{k=1}^{3}\xi_k\left[\sum_{j=1}^{s}(t_k)_j\right]\psi$$
$$T_k\equiv\sum_{j=1}^{s}(t_k)_j,[T_1,T_2]_-=iT_3;\quad\delta\psi=2i\sum_{k=1}^{3}\xi_kT_k\psi$$

Неприводимое представление для группы $SU(2)$: базис

$$B_{jm}=N_{jm}z_1^{j+m}z_2^{j-m},m=-j,-j+1,...,j-1,j$$
$$B'_{jm}=N_{jm}z_1'^{j+m}z_2'^{j-m}=N_{jm}(az_1+bz_2)^{j+m}(-b^*z_1+a^*z_2)^{j-m}$$

Преобразование будет унитарным, если $\sum_{n=-j}^{j}\left|B'_{jn}\right|^2=\sum_{m=-j}^{j}|B_{jm}|^2$. Инвариант преобразования $Z'=WZ:\quad|z_1'|^2+|z_2'|^2=|z_1|^2+|z_2|^2$.

$$\sum_{m=-j}^{j}|B_{jm}|^2=\sum_{m=-j}^{j}N_{jm}^2(z_1^*z_1)^{j+m}(z_2^*z_2)^{j-m}\sim\left(|z_1|^2+|z_2|^2\right)^{2j}$$
$$(a+b)^n=\sum_{k=0}^{n}C_k^na^kb^{n-k}=\sum_{k=0}^{n}\tfrac{n!}{k!(n-k)!}a^kb^{n-k}$$
$$n=2j,k=j+m,n-k=j-m;k=0\to m=-j,k=2j\to m=j$$
$$(a+b)^{2j}=\sum_{m=-j}^{2j}C_{j+m}^{2j}a^{j+m}b^{j-m}=\sum_{m=-j}^{2j}\tfrac{2j!}{(j+m)!(j-m)!}a^{j+m}b^{j-m}.$$

Неприводимое представление для группы $SU(2)$: матрица

$$N_{jm}=\frac{1}{\sqrt{(j+m)!(j-m)!}},B_{jm}=\frac{1}{\sqrt{(j+m)!(j-m)!}}z_1^{j+m}z_2^{j-m}$$

$$\sum_{n=-j}^{j}\left|B'_{jn}\right|^2=\frac{1}{2j!}\left|z'_1\right|^2+\left|z'_2\right|^2=\frac{1}{2j!}\left|z_1\right|^2+\left|z_2\right|^2=\sum_{m=-j}^{j}\left|B_{jm}\right|^2$$

$$B'_{jm}=\sum_n A^j_{nm}B_{jn}=\frac{1}{\sqrt{(j+m)!(j-m)!}}\left(az_1+bz_2\right)^{j+m}\left(-\bar{b}z_1+\bar{a}z_2\right)^{j-m}=$$

$$=\frac{1}{\sqrt{(j+m)!(j-m)!}}\sum_{s_1,s_2}\frac{(j+m)!}{s_1!(j+m-s_1)!}\left(az_1\right)^{j+m-s_1}\left(bz_2\right)^{s_1}\times$$

$$\times\frac{(j-m)!}{s_2!(j-m-s_2)!}\left(-\bar{b}z_1\right)^{j-m-s_2}\left(\bar{a}z_2\right)^{s_2}=$$

$$=\sum_{s_1,s_2}\frac{\sqrt{(j+m)!(j-m)!}(-)^{j-m-s_2}}{s_1!s_2!\left(j+m-s_1\right)!\left(j-m-s_2\right)!}a^{j+m-s_1}\bar{a}^{s_2}b^{s_1}\bar{b}^{j-m-s_2}z_1^{j+m-s_1+j-m-s_2}z_2^{s_1+s_2}$$

$$=\sum_{s_1,s_2}\frac{\sqrt{(j+m)!(j-m)!}(-)^{j-m-s_2}}{s_1!s_2!\left(j+m-s_1\right)!\left(j-m-s_2\right)!}a^{j+m-s_1}\bar{a}^{s_2}b^{s_1}\bar{b}^{j-m-s_2}z_1^{2j-s_1-s_2}z_2^{s_1+s_2}$$

Обозначим $n\equiv j-s_1-s_2;s_1+s_2=j-n,s_2=j-n-s_1,j-m-s_2=n-m+s_1$

$$B'_{jm}=\sum_n\sum_s\frac{\sqrt{(j+m)!(j-m)!}(-)^{n-m+s}}{s!(j+m-s)!(j-n-s)!(n-m+s)!}a^{j+m-s}\bar{a}^{j-n-s}b^s\bar{b}^{n-m+s}z_1^{j+n}z_2^{j-n}$$

$$=\sum_n\sum_s\frac{\sqrt{(j+m)!(j-m)!(j+n)!(j-n)!}}{s!(j+m-s)!(j-n-s)!(n-m+s)!}(-)^{n-m+s}a^{j+m-s}\bar{a}^{j-n-s}b^s\bar{b}^{n-m+s}B_{jn}$$

Покажите, что n меняется от $-j$ до j.

$$A^j_{n,m}=(-)^{n-m}\sum_s(-)^s\frac{\sqrt{(j+m)!(j-m)!(j+n)!(j-n)!}}{s!(j+m-s)!(j-n-s)!(n-m+s)!}\times$$

$$\times a^{j+m-s}\bar{a}^{j-n-s}b^s\bar{b}^{n-m+s}$$

1.
$W=I:a=1,b=0$. Чтобы ушли степени $b:s=0,n=m$, и $A^j_{nm}=\delta(n-m)$.
2.
Каждому W -своя матрица A^j. Если $W_1\to A^j_1$ и $W_2\to A^j_2$, то $W_2W_1\to A^j_2A^j_1$.
3.
Если $a\to -a,b\to -b$, то $(-)^{j+m-s+j-n-s+s+n-m+s}=(-)^{2j}$, и $A^j\to(-)^{2j}A^j$.

24.2.3 Transformations of Minkowski Space

(в теории поля это пишу подробно, тут будет короткое указание.)

Вращение пространства Минковского

Бусты пространства Минковского

24.3 Quantum Chaos: Some Concepts

(когда-то подумаю про это)

24.3.1 Concept of Quantum Chaos

(когда-то подумаю про это, но подробнее - отдельная запись)

24.3.2 Main Models of Quantum Chaos

(когда-то подумаю про это, но подробнее - отдельная запись)

24.3.3 Chaos and the semiclassical limit of quantum mechanics (is the moon there when somebody looks?) by Berry 1

Summary

According to the correspondence principle, the classical world should emerge from the quantum world whenever Planck's constant h is negligible. But the limit $h \to 0$ is mathematically singular. This fact (shared by many physical theories that are limits of other theories) complicates the reduction to classical mechanics. Particular interest attaches to the situation where the classical orbits are chaotic, that is, unpredictable. Then if the system is isolated the corresponding quantum motion (e.g. of a wave-packet) cannot be chaotic; this is the 'quantum suppression of chaos'. Chaos occurs in the world because quantum systems are not isolated: the limit $h \to 0$ is unstable, and the associated quantum interference effects are easily destroyed by tiny uncontrolled influences from the environment, and chaos returns; that is, 'decoherence' suppresses the quantum suppression of chaos. This is illustrated by the chaotic tumbling of Saturn's satellite Hyperion. For isolated systems, there are nevertheless quantal reflections of classical chaos, in the form of borderland phenomena, allowed because the semiclassical limit is singular. These are nonclassical, but emerge as $h \to 0$. Examples are interference associated with focusing (e.g. supernumerary rainbows), and the energy-level statistics of highly excited states, with tantalizing connections to prime numbers and the Riemann hypothesis.

1. Introduction

The question of how chaos in classical mechanics gets reflected in the quantum mechanics of the microworld is slippery and subtle [1-3]. On the one hand, it is known from observations, computations, and mathematical theorems that newtonian mechanics often predicts unpredictability: some systems of forces are so unstable that nearby trajectories separate exponentially fast [4]. This is chaos - the celebrated 'sensitivity to initial conditions'. Chaos is, strictly speaking, a phenomenon defined in the limit of long times, for systems that are confined to a restricted region of space (for example, a particle bouncing in a billiard table in the shape of a stadium). One of the hallmarks of chaos is the lack of periodicity or quasi-periodicity in the time-development of any dynamical variable (for example, the x component of position or the y component of velocity); the mathematical statement of this is that these variables have a continuous spectrum.

On the other hand, the corresponding quantum systems always have discrete (that is, quantized) energy levels, and since the energy spectrum governs the time-development of any dynamical quantity such evolution cannot be chaotic. This is the origin of the often-repeated, and strictly true, assertion that there is no chaos in quantum mechanics. Two awkward questions immediately arise. The first stems from the fact that classical mechanics is supposed to be the limit of quantum mechanics in situations where Planck's constant h can be neglected. This looks like a contradiction, and we ask: what kind of limit is it where a system is not chaotic for any finite value of h, yet is chaotic when $h = 0$? The second question is connected with the recognition that strictly speaking all systems - even our orbiting moon - obey the laws of

quantum mechanics, and yet they are often observed to evolve chaotically (even the moon is slightly chaotic, and other astronomical bodies much more so). We ask: what is the origin of the observed chaos in our macroscopic but strictly quantum world?

My purpose here is to try to answer these questions in the simplest way, that is without formalism. First, though, I draw attention to the fact that the relation between chaos and quantum physics, important enough as it is in its own right, can also be regarded as a microcosm of much larger questions. Our scientific understanding of the world is a patchwork of vast scope; it covers the intricate chemistry of life, the sociology of animal communities, the gigantic wheeling galaxies, and the dances of elusive elementary particles. But it is a patchwork nevertheless, and the different areas do not fit well together. This is the notorious problem of reduction: we might believe that a living organism is described completely by the quantum mechanics of all its molecular (atomic, electronic, nucleonic, quarkish...) parts, but where in its byzantine wavefunction, governed by the Schrödinger equation, is the spark of life? Even if we knew, how could that quantum description extend beyond living cells and individual creatures, to the displays of peacocks and the flocking of birds?

Even within physical science, reduction between different levels of explanation is problematic - indeed, it is almost always so. Chemistry is supposed to have been reduced to quantum mechanics, yet people still argue over the basic question of how quantum mechanics can describe the shape of a molecule. The statistical mechanics of a fluid reduces to its thermodynamics in the limit of infinitely many particles, yet that limit breaks down near the critical point, where liquid and vapour merge, and where we never see a continuum no matter how distantly we observe the particles; the critical state is a fractal, and much theoretical physics of the last forty years has gone into getting a clear understanding of it. The geometrical (newtonian) optics of rays should be the limit of wave optics as the wavelength becomes negligibly small, yet we shall see that the reduction (mathematically similar to that of classical to quantum mechanics) is obstructed by singularities, even when there is no chaos. (A singularity is a place where the smoothness of a mathematical quantity or geometrical pattern is disrupted, for example by the quantity becoming infinite; I will give examples later.)

What follows should not be misconstrued as antireductionist. On the contrary, I am firmly of the view, beautifully expressed recently [5], that all the sciences are compatible and that detailed links can be, and are being, forged between them. But of course the links are subtle, and my emphasis will be on a mathematical aspect of theory reduction that I regard as central, but which cannot be captured by the purely verbal arguments commonly employed in philosophical discussions of reduction.

My contention here will be that many difficulties associated with reduction arise because they involve singular limits [6]. These singularities have both negative and positive aspects: they obstruct the smooth reduction of more general theories to less general ones, but they also point to a great richness of borderland physics between the theories. So, indeed, the problem to be considered here, of chaos in the quantum world, is an example of something grander. But examples are important. To paraphrase the numerical analyst Beresford Parlett: "Only wimps study only the general case. Real scientists study examples".

Before getting started, I must make four points. The first is that although we will be dealing with the limit $h \to 0$, at first encounter this seems meaningless. Planck's constant cannot be set equal to zero, because it is a constant of nature, with a fixed value. And on the other hand, h has dimensions, so its 'fixed' value can be anything, depending on the system of units used. In fact, by 'the semiclassical limit $h \to 0$ ' I will mean 'situations where the dimensionless variable obtained by dividing h by any classical quantity with the same dimensions (action) is negligibly small'.

The second point is that discussions of chaos have been confused by conflating two different questions. The first is: How does classical behaviour (e.g. chaos) emerge in the semiclassical

limit? If the limit $h \to 0$ were not singular, this emergence would be trivial: simply solve the quantum problem, which involves h, then set $h = 0$. But we shall see that the true answer is much more subtle. This first question is important for the intellectual coherence of our description of the physical world, yet in a sense it is backward-looking, since we know the answer: the classical
world has to emerge somehow. The second question, more productive of new physics, is: What nonclassical phenomena emerge as $h \to 0$? This sounds like nonsense, and indeed if the limit were not singular the answer would be: no such phenomena.

The third point is that in discussions of chaos and quantum physics there always lurks a second limit, in addition to $h \to 0$. This is the limit of long times, $t \to \infty$. As mentioned above, it is only in the long-time limit that classical chaos emerges: it takes infinitely long time to verify that a trajectory explores all the possibilities compatible with conservation of energy (and similar quantities), or to determine that two initially infinitesimally close trajectories separate exponentially fast. But the semiclassical and long-time limits do not commute, and thereby hangs much of the difficulty and subtlety associated with our subject.

The fourth point is that there are two questions that were the legitimate focus of attention by most of the other participants at the meeting, but that I will not discuss. One is the relation, if any, that these considerations of quantum chaology bear to theological matters; I am unqualified (and also, as a nonbeliever, unmotivated) to do that. The other is the relation, if any, between quantum chaology and the interpretation of quantum mechanics (measurement, wavepacket reduction, etc); I have some sympathy with the opinion mischievously expressed recently [7] that such interpretation is unnecessary.

24.3.4 Chaos and the semiclassical limit of quantum mechanics (is the moon there when somebody looks?) by Berry 2

2. Singular limits: when one plus one does not make two

To see that singularities in the semiclassical limit are unavoidable, consider the simplest possible situation [8] (where there is no chaos) of two beams of quantum particles, or waves of light, + and - , travelling in opposite directions, and coherent (e.g. created from a common source). The associated waves - complex functions of position and time - are

$$\psi_{\pm}(x,t) = \exp\left\{2\pi \mathrm{i}\left(\pm\frac{x}{\lambda} - vt\right)\right\} \tag{1}$$

where the wavelength λ and frequency v are related to the momentum p
and and energy E of the quantum particles by the de Broglie and Planck laws:

$$\lambda = h/p, \quad v = E/h. \tag{2}$$

Each wave has intensity $|\psi|^2 = 1$.
By linearity (one of the principles of quantum mechanics), the resultant wave is the sum (superposition) of the two, so the (observable) intensity is

$$I(x) = |\psi_+ + \psi_-|^2 = 4\cos^2\left(\frac{2\pi x}{\lambda}\right) \tag{3}$$

This is the simplest representation of interferometry, where x would be distance measured on an observation screen. The oscillatory function (3) describes the interference fringes familiar since their explanation in terms of superposition by Young two centuries ago, and its mathematization by Fresnel (they were studying light, but nowadays the same interference is routinely observed for all quantum particles). Its values oscillate (figure 1a) between zero and 4 , with a spatial period of $\lambda/2$.

Now we ask: what is the classical, or geometrical-optics, limit of this wave? By (2), $h \to 0$ corresponds to fixing the momentum and letting $\lambda \to 0$. Classically (or in geometrical optics) there is no interference, so the intensity resulting from adding two waves, each with unit intensity, should be $I = 2$. But it is not! As $h \to 0$, the intensity (3) oscillates faster and faster (figure 1b), and in the limit it attains all values between zero and 4 in arbitrarily small ranges of x. In fact, (3) has a powerful singularity at $\lambda = 0$ (or $h = 0$), obstructing the smooth passage to the limit. We used to tell ourselves, and our students, that this singular function, and others like it, are mathematical curiosities, of no interest in physics. Now we see that the singularity arises unavoidably when we try to bridge the gap between two of our major theories, in the simplest possible case. For wave intensities, $1 + 1 = 2$ is false, all the way to the classical limit.

And yet we know that, in words attributed to Lord Rayleigh, two candles are twice as bright as one, that is, when waves are irrelevant, one plus one is indeed two. The only way to extract this result from (3) is by averaging. Any external influence that compromises the purity of (3) will have the effect of blurring (3), and in the classical limit this function is infinitely sensitive to blurring. Two possible influences are finite x sensitivity (window size) of the detector, and non-monochromaticity of the beams (finite spreads in wavelength or momentum). Now the average of the function $\cos^2$ is $1/2$, so

$$\langle I(x) \rangle = 4 \left\langle \cos^2 \left(\frac{2\pi x}{\lambda} \right) \right\rangle = 4 \times \frac{1}{2} = 2 \tag{4}$$

which is of course the classical result.

We need a slightly expanded version of (4). The average is over the phase difference χ between the two waves. Imagine the external influences result in a gauss-distributed χ with spread Δ; then

$$\left\langle \cos^2 \chi \right\rangle = \frac{1}{\Delta\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}\chi \cos^2 \chi \exp\left\{ -\frac{\chi^2}{2\Delta^2} \right\} = \frac{1}{2} \left(1 + \exp\left\{ -2\Delta^2 \right\} \right) \tag{5}$$

Phase randomness is very efficient: for phase spread $\Delta = \pi/2$, $\langle \cos^2 \chi \rangle = 0.5003$; for $\Delta = \pi$, $\langle \cos^2 \chi \rangle = 0.500000001$.

So, the correspondence principle does hold, but there has been a price to pay: because of the singularity, classical mechanics emerges not directly, but only after averaging over phase-scrambling effects that can be ascribed to the environment - that is, influences external to the pure quantum wave initially calculated - in modern parlance, decoherence effects. All this to get $1 + 1 = 2$! I cannot resist recalling that in a classic work [9] constructing mathematics from its basis in logic (before Gödel proved that enterprise is doomed), $1 + 1 = 2$ is derived as a theorem, somewhere in the middle of volume 2 .

3. Decoherence and the emergence of chaos

Now, what about chaos? To fix our ideas, consider Hyperion, the sixteenth satellite of the planet Saturn. This body is a potato-shaped rock about as big as New York City ($R \sim 142$ km). To the best of our knowledge, Hyperion is unique in that its rotation is chaotic [10,11]. Under resonant forcing from the big moon Titan, in combination with Saturn's gravity and its own nonsphericity, Hyperion tumbles erratically. The instability has a time-constant (for exponential forgetting of its initial state) of about 100 days, long compared with both its orbital period (21.3 days) and its instantaneous rotation period (about 5 days).

Now consider the rotation of Hyperion, regarded as a quantum object. Its quantized angular momentum J consists of $2\pi J/h \approx 2 \times 10^{58}$ Planck units (see Appendix A for the basis of the estimates given in this section). From this enormous number, together with the correspondence

principle - and with the same modelling as we use for the classical dynamics, where the only forces come from Saturn and Titan - the quantum predictions for the motion ought to coincide with the classical to very high accuracy. Let us see.

It helps to think of the classical motion on the phase space represented by the angular momentum vector $\mathbf{J}$ (whose magnitude is $J = |\mathbf{J}|$); this is the surface of a sphere with polar coordinates θ, ϕ. The motion of the vector $\mathbf{J}$ can be regarded as that of a mechanical system with a single freedom, whose 'coordinate' is the azimuth angle ϕ and whose 'momentum' is $p = J\cos\theta$; therefore phase-space area is area on the sphere, divided by J. For Hyperion, the total available phase-space area is $4\pi J^2/J \approx 10^{58}h$.

If we knew the motion precisely, Hyperion's rotation would be a single point moving on the sphere. But even classically our measurements are not perfectly precise, so the state of Hyperion is a little blurry patch, tiny on the sphere but with an area many times h; call its boundary $B(0)$, evolving into $B(t)$. Chaotic evolution means that the different points on B separate exponentially, so that $B(t)$ develops into a convoluted curve, with tendrils exploring the whole phase sphere. The area enclosed by $B(t)$ remains constant (this is Liouville's theorem); however B 's perimeter length grows exponentially, as $L(t) \approx L(0)\exp(t/T_{\rm c})$, where for Hyperion the chaos time is $T_{\rm c} \approx 100$ days.

Classically, the convolutions get ever more intricate. For a while, the quantum state representing Hyperion follows these convolutions; this is the spreading of the wavepacket, chaos-style. But quantum physics prevents the intricacy - that is, the chaos - from developing forever, because phase-space fine structure is limited by Planck's constant h. Any smaller structure must be blurred. After some time $T_{\rm q}$, the areas of typical tendrils get finer than h; thereafter, classical and quantum evolutions are different. This is the quantum suppression of classical chaos [12-14]. At first thought, $T_{\rm q}$ for astronomical objects must be enormously long, probably irrelevant to any observations on time scales relevant to astronomers - remember that gigantic 10^{58}. Not so. A simple estimate (Appendix A) gives

$$T_{\rm q} \sim T_{\rm c}\log(J/h) \tag{6}$$

For Hyperion, this is

$$T_{\rm q} \sim 100 \text{ days } \times \log\left(10^{58}\right) = 37 \text{ years} \tag{7}$$

- an astonishingly short time, first calculated in a similar way by Ronald Fox (private communication).

Now, the chaotic rotation of Hyperion was discovered less than 37 years ago, but nobody thinks that after the year 2020 astronomers will begin to see quantum effects - specifically the calming of Hyperion's instability and its replacement by some more moderate multiply periodic motion. And indeed, the predicted quantum suppression of chaos is itself suppressed, and classicality restored, by another quantum effect. This is decoherence. It arises from the fact that Hyperion is not isolated.

At the very least, seeing Hyperion involves photons from the sun, arriving unpredictably. We would never think to include these photons in
the calculation of Hyperion's dynamics, because their energy is so minuscule: 4×10^{-19} J for a visible photon, as compared with $2 \times 10^{+19}$ J for Hyperion's rotational energy. On the other hand, their energy is vast in comparison with the energy spacing 10^{-39} J of Hyperion's quantum rotational levels, so a quantum effect from these photons is conceivable.

The proper way to calculate this effect would be to enlarge the physical system to include not just Hyperion in the field of Saturn and Titan but also the sun's radiation field, and formally eliminate the radiation variables (by tracing over them), to get a modified quantum mechanics

involving only Hyperion's dynamics. In recent years powerful formalisms have been developed for doing this [15, 16], and have been applied to the situation where there is classical chaos [17-19]. Rather than repeat these arguments here, I will first estimate the effects of decoherence in a bare-handed way, by treating the environment as a random time-dependent modification of Hyperion's hamiltonian - a kick from each impact of a photon from the sun. In Appendix B I give a slightly more formal treatment, but still incorporating what John Polkinghorne calls 'the patter of photons' as an external influence, rather than a constituent of a composite system.

We begin by noting that the quantum suppression of chaos involves the interference of waves and therefore their phases (in some situations this is analogous to Anderson localization in solids [20]). Therefore the suppression can be easily - and quickly - destroyed by decoherence from external influences. The change in Hyperion's angular momentum resulting from the random impact (impulsive torque) of a single visible photon (wavelength λ) is $\Delta J \sim (h/\lambda)R$. This impact will change the total phase of Hyperion's wavefunction. And, with even slight convolutions of B, so there is more than one classical contribution to the wavefunction for some azimuth values ϕ, it will also (by about the same amount) change the phase difference between these contributions. The change (associated with the component of $\mathbf{\Delta J}$ parallel to $\mathbf{J}$, which spins up Hyperion and swells the sphere and therefore also the convolutions of B on it) is

$$\Delta J/h \sim (h/\lambda)R/h = R/\lambda \sim 10^{11} \tag{8}$$

This uncontrollable phase shift between the waves associated with any two classical contributions, acting according to (5), is overwhelmingly sufficient to induce decoherence, and so suppress the suppression of chaos - and just from a single photon. In the stream of sunlight (flux˜10 Wm $^{-2}$), photons arrive at a rate of one every 10^{-30} s, so decoherence occurs extremely fast. Stretching this argument, we can estimate the decoherence time $T_{\rm d}$ for the stream of photons from the sun to disturb the phase by about 2π radians:

$$T_{\rm d} \sim 10^{-53} \text{ s} \tag{9}$$

Do not take the precise value of this number seriously. The foregoing is very far from a proper calculation of the decoherence effect for Hyperion. But the extreme smallness of $T_{\rm d}$ should be taken very seriously. It shows that an external disturbance so small that its effect on a system's dynamics is negligible (one photon, or a tiny fraction of a photon) can nevertheless dramatically and effectively instantaneously influence the kinematics of its quantum state - and more strongly as the classical limit is approached. Decoherence - the generalization of the $1 + 1 = 2$ calculation of the previous section - emerges as a dominant physical effect, allowing classical chaos to persist [17-19].

I chose Hyperion's chaos to dramatize the way in which uncontrolled environmental influences can induce quantal decoherence. In fact, when applied in such extreme situations the decoherence argument has nothing to do with chaos per se, but to classicalization: since $T_{\rm d} \ll T_{\rm c}$, the destruction of quantum interference occurs long before chaos develops. So the claim sometimes made, that chaos amplifies quantum indeterminacy, is misleading. The situation is more subtle: chaos magnifies any uncertainty, but in the quantum case h has a smoothing effect, which would suppress chaos if this suppression were not itself suppressed by externally-induced decoherence, that restores classicality (including chaos if the classical orbits are unstable).

The calculation in Appendix B shows this decoherence-induced classicalization more clearly for the illustrative example of Hyperion; very recently, a more general and formal argument for the universality of the phenomenon has been given [21]. At the opposite extreme from Hyperion are the humble 2-state systems, where decoherence, and the related inhibition of quantum transitions through the quantum Zeno effect, can be explored in detail [22-29].

24.3.5 Chaos and the semiclassical limit of quantum mechanics (is the moon there when somebody looks?) by Berry 3

4. Emergent semiclassical phenomena

The example of Hyperion addressed the first of the two commonlyconflated questions mentioned near the end of the Introduction, namely the emergence of classical effects - specifically, chaos - as $h \to 0$. Now, with two examples, we consider the more interesting question of what nonclassical effects emerge and persist in the limit $h \to 0$. The first does not involve chaos; the second does. Both of these emergent phenomena are delicate, in the sense that their detection requires magnification that increases as h gets smaller; this contrasts with more familiar examples of macroscopic quantum phenomena (superfluidity, superconductivity, the impenetrability of matter in bulk...).

Corresponding to a quantum scattering wavefunction (for example of a beam of atoms striking a target of other atoms, or electrons in an electron microscope) or to a field of diffracted light waves (for example sunlight encountering a raindrop), is a family of trajectories. These are the orbits of massive particles, or light rays. (Even a localized wavepacket corresponds to a family, rather than a single trajectory, because its localization cannot be perfect.)

Now, a family of trajectories possesses a holistic property not inherent in any individual trajectory, namely focusing. In three dimensions, focusing usually occurs on surfaces, and in two dimensions, on lines. These are the envelopes of the family of trajectories. They are called caustics. Caustics are the singularities of ray (geometrical, classical) theory [30, 31]. On them, the ray intensity rises to infinity.

They are the brightest places in the field. Examples are rainbows (angular focusing of sunlight refracted and reflected by raindrops, and their analogues in atomic and molecular scattering) and the patterns of light dancing on the bottom of a swimming-pool. In our eyes, microscopes and cameras, the images of each point are also formed by focusing, but of a very special kind, namely the non-generic points fashioned by evolution or lensmakers' art, rather than the surfaces and lines occurring when there is no symmetry. Caustics are important.

But they are nonexistent! Close examination, on the scale of the wavelength, dissolves the singularities, and reveals that they are decorated by intricate and beautiful interference patterns. These can be understood by an application of the same mathematics, developed in the 1960s and 1970s, that enables the different caustic singularities to be classified. This is the celebrated and (in other contexts) notorious catastrophe theory [32, 33]. The diffraction catastrophes [31, 34, 35] are emergent semiclassical (more generally, short-wave) phenomena, with many applications throughout mathematics as well as physics (they describe the supernumerary arcs sometimes seen just inside the main rainbow, that were impossible to explain using ray theory). Although they are contained in wave equations (Schrödinger's, Maxwell's), they were not derived by the reductionist approach of starting with solutions of wave equations, but by top-down methods, starting with the caustic singularities of ray physics; only later were the full connections with wave equations elucidated, and consilience [5] established.

Before getting to the second example, I digress to point out that the caustics story extends deep into wave physics, and in a way that nicely illustrates the role of singularities. Wave physics dissolves the caustic singularities of geometrical optics. But wave physics has singularities of its own, complementary to caustics; these are the singularities of phase the new quantity introduced in the generalization from rays to waves. The singularities are the dislocation lines [31, 36-38] (so called because of their close analogy with dislocations in crystals), where the phase is singular and the intensity is zero. Dislocations are fine-scale features of waves; they are now beginning to be investigated in detail in optical
experiments with interfering laser beams [39,40]. They are optical singularities in the approximation where light is regarded as a scalar wave. But light is not a scalar wave; its vector nature

allows for polarization. And in the passage from scalar to vector, the dislocations are dissolved, and replaced by yet other singularities, of the pattern of field vectors: lines again, but where the polarization is purely circular or purely linear [41-43]. At each stage, generalization to a deeper theory dissolves the singularities of the old theory, and replaces them by new ones.

Now we return to chaos, with our second example, and consider the conventional quantum mechanics of isolated systems, mindful of the fact that as the classical limit is approached the criteria for effective isolation become more stringent. An isolated bounded system possesses discrete energy levels. For fixed energy, the semiclassical limit corresponds to highly excited states, so we expect these to reflect the nature of the corresponding classical trajectories, in particular their chaology. And so it turns out, in a remarkable example of an asymptotically emergent phenomenon associated with a singular limit.

First, there is an obvious way in which the classical limit is singular. Between the classical energy continuum and the quantum discontinuum is a logically unbridgeable gap. In philosophers' parlance, the two theories are incommensurable. In practice, the incommensurability is inconsequential, because any spectroscope has finite resolution, and under sufficiently semiclassical conditions the discrete levels (spacing h^D for systems with D freedoms) cannot be discriminated. Beyond this, we can imagine studying the details of the semiclassical spectrum by performing a mental magnification to keep the average level spacing unity.

Now it is possible to ask whether the thus-magnified spectrum is qualitatively different for a classically integrable (regular, non-chaotic) system and for a chaotic one. For example, the much-investigated quantum dots can be caricatured as quantum billiards, that is electrons moving freely in planar regions with specular reflection at the boundary walls; square or circular boundaries generate classically regular motion, a
stadium-shaped wall generates chaos. (Other chaotic systems that have been studied experimentally include hydrogen atoms in very strong magnetic fields, and the vibrations of molecules whose atoms are anharmonically coupled.)

These spectra display universality. There is a sense in which the spectra of all quantum systems whose classical mechanics is chaotic are the same, and similarly for integrable systems [2, 44-46]. The universality does not extend to the positions of the individual levels: of course these are different for different systems in each class. It is to the statistics of the levels that universality applies. Statistics are natural in the semiclassical limit, since there are many levels in a classically small energy interval. Spectral statistics has become a richly elaborated subject [47], of which the merest sketch must suffice here.

Consider one of the simplest statistics of the magnified spectrum (where the mean spacing is unity), namely the probability $P(S)$ that neighbouring levels have spacing S. For almost all integrable systems with more than one freedom,

$$P(S) = \exp(-S) \text{ (integrable)}; \tag{10}$$

this is the negative exponential characteristic of Poisson-distributed 'events' (levels); in particular, the most probable spacing is $S = 0$, indicating clustering of the levels [44]. It is a little strange at first encounter that regular classical motion coresponds to a random quantum spectrum, but it is so.

For chaotic classical motion, the level spacings distribution is very different, and closely approximated by the Wigner distribution [1,48]

$$P(S) = \frac{1}{2}\pi S \exp\left(-\frac{1}{4}\pi S^2\right) \text{ (chaotic)}. \tag{11}$$

This is the statistic characteristic of the eigenvalues of random matrices [49, 50]. Note that $P(0) = 0$, indicating repulsion of levels, in contrast to the clustering of (10).

I have simplified matters. There are actually three universality classes for classically chaotic quantum spectra. Equation (10) applies when there is time-reversal symmetry, when the particles have integer spin (bosons) or where spin plays no part (as in electrons in quantum billiards). The other universalities apply when there is time-reversal symmetry for fermions [51], and when there is no time-reversal symmetry [52-54].

It is one thing to identify universality classes, by computer experiments inspired by intuition, or (now) by laboratory experiment, but quite another to provide a theoretical explanation of the universality. However, this has now been achieved, both in broad outline and in many details [55-57]. It turns out that the quantum spectral universality is begotten by a universality of the classical mechanics, connected with the distribution of very long periodic orbits [58, 59]. And in one of those unexpected connections that make theoretical physics so delightful, the quantum chaology of spectra turns out to be deeply connected to the arithmetic of prime numbers, through the celebrated zeros of the Riemann zeta function: the zeros mimic quantum energy levels of a classically chaotic system. The connection is not only deep but also tantalizing, since its basis is still obscure - though it has been fruitful both for mathematics and physics [60-66].

It is important to emphasize why spectral universality is an emergent nonclassical semiclassical phenomenon. It is nonclassical because it is a property of discrete energy levels, which have no classical counterpart. It is semiclassically emergent because only as $h \to 0$ are there many levels in a classically small interval - it is impossible to calculate statistics using only the ground state. And only the singular nature of the semiclassical limit allows such nonclassical phenomena to emerge without paradox.

Appendix A

Caricaturing Hyperion as a homogeneous sphere with radius $R(= 142\,\mathrm{km})$ and mass $M\,(= 1.77 \times 10^{19}\ \mathrm{kg})$, its moment of inertia is $I = 2MR^2/5$, and from its rotational angular speed $\Omega_\mathrm{H} \sim 2\pi/(5\ \mathrm{days}\ )$ follows the angular momentum

$$J = I\Omega_\mathrm{H} = \frac{2}{5}MR^2\Omega_\mathrm{H} \tag{A1}$$

and thence the number $N = 2\pi J/h = 2\times 10^{58}$ given in the text, of Planck units in Hyperion's angular momentum.

For the estimate of T_q (equations 6 and 7), we imagine the boundary of the patch representing Hyperion's classical state evolving into tendrils each of area h. Since the total area of the angular-momentum sphere (phase space) is $4\pi J$, the number of such tendrils is about N, and their total perimeter is $L\,(T_\mathrm{q}) \sim N\mathrm{x}$ (radius of J sphere) $\sim N\sqrt{J} = N^{3/2}\sqrt{h}$; the initial perimeter is $L(0) \sim \sqrt{J} = \sqrt{(Nh)}$. Solving the chaos equation

$$L\,(T_\mathrm{q}) = L(0)\exp\,(T_\mathrm{q}/T_\mathrm{c}) \tag{A2}$$

for T_q now gives (6) and (7).

To estimate the spacing of Hyperion's rotational eigenenergies E_N, we use

$$E_N = \frac{J^2}{2I} = \frac{N^2h^2}{8\pi^2 I} \tag{A3}$$

whence

$$\Delta E_N \equiv E_{N+1} - E_N = \frac{Nh^2}{4\pi^2 I} = \frac{Jh}{2\pi I} = \frac{h\Omega_\mathrm{H}}{2\pi} \tag{A4}$$

This gives $\Delta E_N \sim 10^{-39}$ J as stated in the text.

Finally, to estimate the decoherence time T_d we start with the energy of sunlight reaching unit area of Hyperion each second. This is about $P = 10\mathrm{Wm}^{-2}$, since $1000\mathrm{Wm}^{-2}$ reaches the

earth and Saturn is about 10 times further from the Sun. The total power reaching Hyperion is thus $\pi R^2 P$; thence the number of photons (frequency v) reaching hyperion in $T_{\rm d}$ is $N_{\rm p} \sim \pi R^2 P T_{\rm d}/hv$. These give random impacts, so the total phase change is $\sqrt{N_{\rm p}}$ times the value in (8), and this must be of order unity, leading to

$$T_{\rm d} \sim \frac{hc\lambda}{\pi R^4 P} \tag{A8}$$

and thence to (9).

Appendix B

My aim here is to use a simple model to get an expression for the 'decoherence factor' that describes explicitly how impacts from photons 'classicalize' Hyperion's rotation, by causing the density matrix, in the representation corresponding to Hyperion's angular position, to become diagonal very rapidly.

On the very small time scales associated with the onset of decoherence, Hyperion's chaotic tumbling is irrelevant, so it suffices to treat the rotation by a single angle θ, with associated angular momentum component J. Let a photon with momentum p strike Hyperion with impact parameter $b(-R \le b \le R)$, and the the reflectivity be r. This will change J by

$$\Delta J = pb(1-r) \tag{B1}$$

A classical hamiltonian incorporating these impacts (denoted by subscripts i) is

$$H = \frac{J^2}{2I} + \theta \sum_i \Delta J_i \delta\left(t - t_i\right) \tag{B2}$$

(H is not periodic in θ, but in the present context θ can be considered as living on the covering space consisting of the whole real line.)

Quantally, the variables θ and J become operators $\hat{\theta}$ and $\hat{J}$, and the evolution of a state $|\psi(t)\rangle$ over the interval $\tau_i = t_{i+1} - t_i \, (\sim 10^{-30}$ s) between the successive impacts is determined (from the Schrödinger equation corresponding to (B2)) by the unitary evolution operator

$$U_i = \exp\left\{-\mathrm{i}\hat{\theta}\Delta J_i/\hbar\right\} \exp\left\{-\mathrm{i}\hat{J}^2\tau_i/(2I\hbar)\right\}. \tag{B3}$$

We apply this in the position representation, for wavepackets $\psi(\theta,t) \equiv \langle\theta \mid \psi(t)\rangle$ that are classically narrow (corresponding to an accurate specification of Hyperion's rotation) and correspond to rotation with average angular momentum J, yet wide enough to neglect the spreading of the wavepacket during the tiny interval τ_i between photon impacts. These conditions are very easy to justify for a planetary wavepacket, as can be confirmed by exact calculations on a gaussian model. Then the evolution is, approximately,

$$\begin{aligned}\psi\left(\theta, t_{i+1}\right) &= \exp\left\{-\mathrm{i}\theta\Delta J_i/\hbar\right\} \langle\theta| \exp\left\{-\mathrm{i}\hat{J}^2\tau_i/(2I\hbar)\right\} |\psi\left(t_i\right)\rangle \\ &\approx \exp\left\{-\mathrm{i}\theta\Delta J_i/\hbar\right\} \exp\left\{-\mathrm{i}J^2\tau_i/(2I\hbar)\right\} \psi\left(\theta, t_i\right)\end{aligned} \tag{B4}$$

Expressing this in terms of the density matrix $\hat{\rho}_i = |\psi\left(t_i\right)\rangle \langle\psi\left(t_i\right)|$ gives, for the evolution after N impacts,

$$\langle\theta|\hat{\rho}_{i+N}\,|\theta'\rangle \approx \exp\left\{-\mathrm{i}\left(\theta-\theta'\right)\sum_{m=i}^{i+N}\Delta J_m/\hbar\right\} \langle\theta|\hat{\rho}_i\,|\theta'\rangle \tag{B5}$$

Now comes the central step: averaging the exponential factor over the random impacts. In a time T during which there are many impacts (which can still be macroscopically extremely short), the exponent is a gaussian random variable. With this observation, and introducing the average photon frequency ω, the decoherence factor can be written

$$F(\theta,\theta',T) = \left[\exp\left[-\mathrm{i}(\theta-\theta')\sum_{i=1}^{N} p_i b_i (1-r_i)/\hbar\right]\right]_{\mathrm{av}} \tag{B6}$$
$$= \exp\left\{-A\omega T(\theta-\theta')^2\right\}$$

where the dimensionless decoherence amplification constant A, expressed in terms of the power P striking unit area of Hyperion, is

$$A \sim \frac{PR^4}{hc^2} \sim 10^{38} \tag{B7}$$

The enormous value of A, together with (B6), ensures that in even the shortest macroscopically significant time T the off-diagonal elements of the density matrix are negligible for any difference $\theta-\theta'$ in Hyperion's angular position that is large enough to conceivably be measured. For a more general version of (B6), see equation (3) of reference [21].

Figure caption

Figure 1. Graphs of the intensity interference function (3) for (a) $\lambda = 0.5$, (b) $\lambda = 0.05$, illustrating the approach to the singular limit $\lambda = 0$, where the intensity takes all values between 0 and 4 .

24.4 Other Fundamental Ideas

24.4.1 Wigner Function in QM (????)

(??? I am not sure, which will I write here)

Wigner function formalism in Quantum mechanics

(??? видимо, хорошие преобразования, с вектором Римана-Силберштейна как-то связано. В ЭД мб его пойму.)

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https://nbi.ku.dk/english/theses/bachelor-theses/jon-brogaard/Jon_Brogaard_Bachelorthesis_2015.pdf

- The RS vector is a natural starting point to introduce the Wigner function for the photon through the standard definition adopted from quantum mechanics

$$W_{ij}(\mathbf{r},\mathbf{k},t) = \int d^3 s e^{-i\mathbf{k}\cdot\mathbf{s}} F_i(\mathbf{r}+\mathbf{s}/2,t) F_j^*(\mathbf{r}-\mathbf{s}/2,t)$$

$$W_{ij} = w_{ij} + \frac{c}{2i}\epsilon_{ijk}u_k$$

$$\partial_t w_{ij} = -c\epsilon_{ilk}k_l w_{kj} - c\epsilon_{jlk}k_l w_{ki} - \frac{c^2}{2}\left(\nabla_i u_j + \nabla_j u_i - \delta_{ij}\nabla_k u_k\right)$$

$$\partial_t u_i = -c\epsilon_{ijk}k_j u_k - \frac{1}{2}\left(\nabla_j w_{ij} - \nabla_i w_{jj}\right)$$

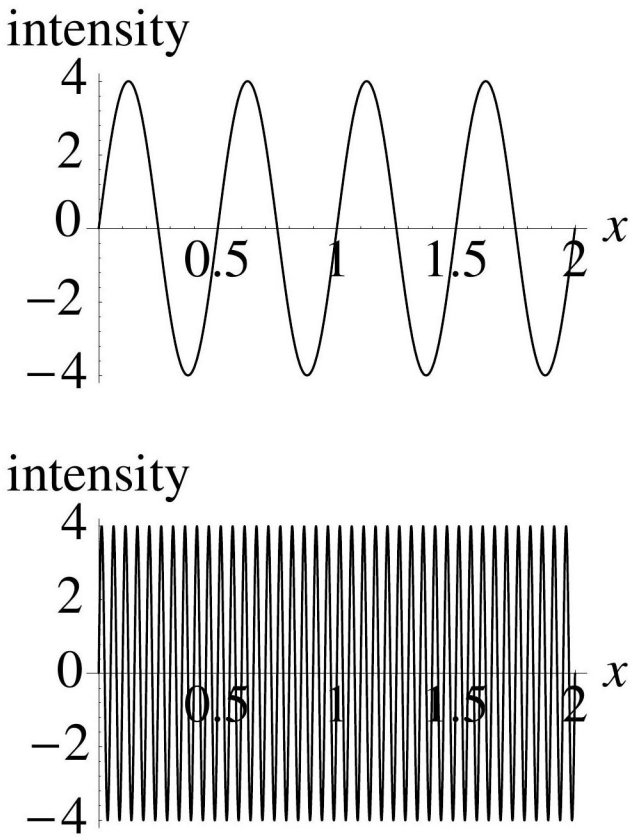

Figure 1. Graphs of the intensity interference function (3) for (a) $\lambda = 0.5$, (b) $\lambda = 0.05$, illustrating the approach to the singular limit $\lambda = 0$, where the intensity takes all values between 0 and 4 .

24.5 Dirac's Quantization Method

24.5.1 Overview of Dirac's Quantization Method

Is Dirac's quantization Method really useful?

(???? I don't know it, it is an important question)

Examples of real applications of Dirac's quantization

(??? never heard that it was used)

24.5.2 Dirac's Lecture 1: The Hamilton Method

I'm very happy to be here at Yeshiva and to have this chance to talk to you about some mathematical methods that I have been working on for a number of years. I would like first to describe in a few words the general object of these methods.

In atomic theory we have to deal with various fields. There are some fields which are very familiar, like the electromagnetic and the gravitational fields; but in recent times we have a number of other fields also to concern ourselves with, because according to the general ideas of De Broglie and Schrödinger every particle is associated with waves and these waves may be considered as a field. So we have in atomic physics the general problem of setting up a theory of various fields in interaction with each other. We need a theory conforming to the principles of quantum mechanics, but it is quite a difficult matter to get such a theory.

One can get a much simpler theory if one goes over to the corresponding classical mechanics, which is the form which quantum mechanics takes when one makes Planck's constant $\hbar$ tend to zero. It is very much easier to visualize what one is doing in terms of classical

mechanics. It will be mainly about classical mechanics that I shall be talking in these lectures.

Now you may think that that is really not good enough, because classical mechanics is not good enough to describe Nature. Nature is described by quantum mechanics. Why should one, therefore, bother so much about classical mechanics? Well, the quantum field theories are, as I said, quite difficult and so far, people have been able to build up quantum field theories only for fairly simple kinds of fields with simple interactions between them. It is quite possible that these simple fields with the simple interactions between them are not adequate for a description of Nature. The successes which we get with quantum field theories are rather limited. One is continually running into difficulties and one would like to broaden one's basis and have some possibility of bringing more general fields into account. For example, one would like to take into account the possibility that Maxwell's equations are not accurately valid. When one goes to distances very close to the charges that are producing the fields, one may have to modify Maxwell's field theory so as to make it into a nonlinear electrodynamics. This is only one example of the kind of generalization which it is profitable to consider in our present state of ignorance of the basic ideas, the basic forces and the basic character of the fields of atomic theory.

In order to be able to start on this problem of dealing with more general fields, we must go over the classical theory. Now, if we can put the classical theory into the Hamiltonian form, then we can always apply certain standard rules so as to get a first approximation to a quantum theory. My talks will be mainly concerned with this problem of putting a general classical theory into the Hamiltonian form. When one has done that, one is well launched onto the path of getting an accurate quantum theory. One has, in any case, a first approximation.

Of course, this work is to be considered as a preliminary piece of work. The final conclusion of this piece of work must be to set up an accurate quantum theory, and that involves quite serious difficulties, difficulties of a fundamental character which people have been worrying over for quite a number of years. Some people are so much impressed by the difficulties of passing over from Hamiltonian classical mechanics to quantum mechanics that they think that maybe the whole method of working from Hamiltonian classical theory is a bad method. Particularly in the last few years people have been trying to set up alternative methods for getting quantum field theories. They have made quite considerable progress on these lines. They have obtained a number of conditions which have to be satisfied. Still I feel that these alternative methods, although they go quite a long way towards accounting for experimental results, will not lead to a final solution to the problem. I feel that there will always be something missing from them which we can only get by working from a Hamiltonian, or maybe from some generalization of the concept of a Hamiltonian. So I take the point of view that the Hamiltonian is really very important for quantum theory.

In fact, without using Hamiltonian methods one cannot solve some of the simplest problems in quantum theory, for example the problem of getting the Balmer formula for hydrogen, which was the very beginning of quantum mechanics. A Hamiltonian comes in therefore in very elementary ways and it seems to me that it is really quite

curritial to work from a Hamiltonian; so I want to talk 10. you about how far one can develop Hamiltonian methods.

I would like to begin in an elementary way and I take as my starting point an action principle. That is to say, I assume that there is an action integral which depends on the motion, such that, when one varies the motion, and puts down the conditions for the action integral to be stationary, one gets the equations of motion. The method of starting from an action principle

has the one great dvantage, that one can easily make the theory conform to the principle of relativity. We need our atomic theory to conform to relativity because in general we are dealing with particles moving with high velocities.

If we want to bring in the gravitational field, then we have to make our theory conform to the general principle of relativity, which means working with a space-time which is not flat. Now the gravitational field is not very important in atomic physics, because gravitational forces are extremely weak compared with the other kinds of forces which are present in atomic processes, and for practical purposes one can neglect the gravitational field. People have in recent years worked to some extent on bringing the gravitational field into the quantum theory, but I think that the main object of this work was the hope that bringing in the gravitational field might help to solve some of the difficulties. As far as one can see at present, that hope is not realized, and bringing in the gravitational field seems to add to the difficulties rather than remove them. So that there is not very much point at present in bringing gravitational fields into atomic theory. However, the methods which I am going to describe are powerful mathematical methods which

would be available whether one brings in the gravitational field or not.

We start off with an action integral which I denote by

$$I = \int L dt \tag{1-1}$$

It is expressed as a time integral, the integrand L being the Lagrangian. So with an action principle we have a Lagrangian. We have to consider how to pass from that Lagrangian to a Hamiltonian. When we have got the Hamiltonian, we have made the first step toward getting a quantum theory.

You might wonder whether one could not take the Hamiltonian as the starting point and short-circuit this work of beginning with an action integral, getting a Lagrangian from it and passing from the Lagrangian to the Hamiltonian. The objection to trying to make this short-circuit is that it is not at all easy to formulate the conditions for a theory to be relativistic in terms of the Hamiltonian. In terms of the action integral, it is very easy to formulate the conditions for the theory to be relativistic: one simply has to require that the action integral shall be invariant. One can easily construct innumerable examples of action integrals which are invariant. They will automatically lead to equations of motion agreeing with relativity, and any developments from this action integral will therefore also be in agreement with relativity.

When we have the Hamiltonian, we can apply a standard method which gives us a first approximation to a quantum theory, and if we are lucky we might be able to go on and get an accurate quantum theory. You might

again wonder whether one could not short-circuit that work to some extent. Could one not perhaps pass directly from the Lagrangian to the quantum theory, and shortcircuit altogether the Hamiltonian? Well, for some simple examples one can do that. For some of the simple fields which are used in physics the Lagrangian is quadratic in the velocities, and is like the Lagrangian which one has in the non-relativistic dynamics of particles. For these examples for which the Lagrangian is quadratic in the velocities, people have devised some methods for passing directly from the Lagrangian to the quantum theory. Still, this limitation of the Lagrangian's being quadratic in the velocities is quite a severe one. I want to avoid this limitation and to work with a Lagrangian which can be quite a general function of the velocities. To get a general formalism which will be applicable, for example, to the non-linear electrodynamics which I mentioned previously, I don't think one can in any way shortcircuit the route of starting with an action integral, getting a Lagrangian, passing from the Langrangian to the Hamiltonian, and then passing from the Hamiltonian to the quantum theory. That is the route which I want to discuss in this course of lectures.

In order to express things in a simple way to begin with, I would like to start with a dynamical theory involving only a finite number of degrees of freedom, such as you are familiar with in particle dynamics. It is then merely a formal matter to pass from this finite number of degrees of freedom to the infinite number of degrees of freedom which we need for a field theory.

Starting with a finite number of degrees of freedom, we have dynamical coordinates which I denote by q.

The general one is $q_n, n = 1, \cdots, N, N$ being the number of degrees of freedom. Then we have the velocities $dq_n/dt = \dot{q}_n$. The Lagrangian is a function $L = L(q, \dot{q})$ of the coordinates and the velocities.

You may be a little disturbed at this stage by the importance that the time variable plays in the formalism. We have a time variable t occurring already as soon as we introduce the Lagrangian. It occurs again in the velocities, and all the work of passing from Lagrangian to Hamiltonian involves one particular time variable. From the relativistic point of view we are thus singling out one particular observer and making our whole formalism refer to the time for this observer. That, of course, is not really very pleasant to a relativist, who would like to treat all observers on the same footing. However, it is a feature of the present formalism which I do not see how one can avoid if one wants to keep to the generality of allowing the Lagrangian to be any function of the coordinates and velocities. We can be sure that the contents of the theory are relativistic, even though the form of the equations is not manifestly relativistic on account of the appearance of one particular time in a dominant place in the theory.

Let us now develop this Lagrangian dynamics and pass over to Hamiltonian dynamics, following as closely as we can the ideas which one learns about as soon as one deals with dynamics from the point of view of working with general coordinates. We have the Lagrangian equations of motion which follow from the variation of the action integral:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_n}\right) = \frac{\partial L}{\partial q_n} \tag{1-2}$$

To go over to the Hamiltonian formalism, we introduce the momentum variables p_n, which are defined by

$$p_n = \frac{\partial L}{\partial \dot{q}_n} \tag{1-3}$$

Now in the usual dynamical theory, one makes the assumption that the momenta are independent functions of the velocities, but that assumption is too restrictive for the applications which we are going to make. We want to allow for the possibility of these momenta not being independent functions of the velocities. In that case, there exist certain relations connecting the momentum variables, of the type $\phi(q, p) = 0$.

There may be several independent relations of this type, and if there are, we distinguish them one from another by a suffix $m = 1, \cdots, M$, so we have

$$\phi_m(q, p) = 0. \tag{1-4}$$

The q 's and the p 's are the dynamical variables of the Hamiltonian theory. They are connected by the relations (1-4), which are called the primary constraints of the Hamiltonian formalism. This terminology is due to Bergmann, and I think it is a good one.

Let us now consider the quantity $p_n\dot{q}_n - L$. (Whenever there is a repeated suffix I assume a summation over all values of that suffix.) Let us make variations in the variables q and $\dot{q}$, in the coordinates and the velocities. These variations will cause variations to occur in the momentum variables p. As a result of these variations, $\delta\left(p_n\dot{q}_n - L\right)$

$$= \delta p_n \dot{q}_n + p_n \delta \dot{q}_n - \left(\frac{\partial L}{\partial q_n}\right) \delta q_n - \left(\frac{\partial L}{\partial \dot{q}_n}\right) \delta \dot{q}_n$$
$$= \delta p_n \dot{q}_n - \left(\frac{\partial L}{\partial q_n}\right) \delta q_n \tag{1-5}$$

by (1-3). Now you see that the variation of this quantity $p_n \dot{q}_n - L$ involves only the variation of the q 's and that of the p 's. It does not involve the variation of the velocities. That means that $p_n \dot{q}_n L -$ can be expressed in terms of the q 's and the p 's, independent of the velocities. Expressed in this way, it is called the Hamiltonian H.

However, the Hamiltonian defined in this way is not uniquely determined, because we may add to it any linear combination of the ϕ 's, which are zero. Thus, we could go over to another Hamiltonian

$$H^* = H + c_m \phi_m, \tag{1-6}$$

where the quantities c_m are coefficients which can be any function of the q 's and the p 's. H^* is then just as good as H; our theory cannot distinguish between H and H^*. The Hamiltonian is not uniquely determined.

We have seen in (1-5) that

$$\delta H = \dot{q}_n \delta p_n - \left(\frac{\partial L}{\partial q_n}\right) \delta q_n$$

This equation holds for any variation of the q 's and the p 's subject to the condition that the constraints (1-4) are preserved. The q 's and the p 's cannot be varied independently because they are restricted by (1-4), but for any variation of the q 's and the p 's which preserves these conditions, we have this equation holding. From the general method of the calculus of variations applied to a variational equation with constraints of this kind, we deduce
and

$$\dot{q}_n = \frac{\partial H}{\partial p_n} + u_m \frac{\partial \phi_m}{\partial p_n} \tag{1-7}$$
$$-\frac{\partial L}{\partial q_n} = \frac{\partial H}{\partial q_n} + u_m \frac{\partial \phi_m}{\partial q_n} \tag{9}$$

$$\text{or} \quad p_n = -\frac{\partial H}{\partial q_n} - u_m \frac{\partial \phi_m}{\partial q_n}, \tag{1-8}$$

with the help of (1-2) and (1-3), where the u_m are unknown coefficients. We have here the Hamiltonian equations of motion, describing how the variables q and p vary in time, but these equations involve unknown coefficients u_m.

It is convenient to introduce a certain formalism which enables one to write these equations briefly, namely the Poisson bracket formalism. It consists of the following: If we have two functions of the q 's and the p 's, say $f(q,p)$ and $g(q,p)$, they have a Poisson bracket $[f,g]$ which is defined by

$$[f,g] = \frac{\partial f}{\partial q_n}\frac{\partial g}{\partial p_n} - \frac{\partial f}{\partial p_n}\frac{\partial g}{\partial q_n} \tag{1-9}$$

The Poisson brackets have certain properties which follow from their definition, namely $[f,g]$ is antisymmetric in f and g :

$$[f, g] = -[g, f] \tag{1-10}$$

it is linear in either member:

$$[f_1 + f_2, g] = [f_1, g] + [f_2, g]\,, \text{ etc.} \tag{1-11}$$

and we have the product law,

$$[f_1 f_2, g] = f_1\,[f_2, g] + [f_1, g]\,f_2 \tag{1-12}$$

Finally, there is the relationship, known as the 7 acobi Identity, connecting three quantities:

$$[f, [g, h]] + [g, [h, f]] + [h, [f, g]] = 0. \tag{1-13}$$

With the help of the Poisson bracket, one can rewrite

[10]

the equations of motion. For any function g of the q 's and the p 's, we have

$$\dot{g} = \frac{\partial g}{\partial q_n}\dot{q}_n + \frac{\partial g}{\partial p_n}\dot{p}_n \tag{1-14}$$

If we substitute for q_n and p_n their values given by (1-7) and (1-8), we find that (1-14) is just

$$\dot{g} = [g, H] + u_m\,[g, \phi_m] \tag{1-15}$$

The equations of motion are thus all written concisely in the Poisson bracket formalism.

We can write them in a still more concise formalism if we extend the notion of Poisson bracket somewhat. As I have defined Poisson brackets, they have a meaning only for quantities f and g which can be expressed in terms of the q 's and the p 's. Something more general, such as a general velocity variable which is not expressible in terms of the q 's and p 's, does not have a Poisson bracket with another quantity. Let us extend the meaning of Poisson brackets and suppose that they exist for any two quantities and that they satisfy the laws (1-10), $(1-11), (1-12)$, and (1-13), but are otherwise undetermined when the quantities are not functions of the q 's and p 's.

Then we may write (1-15) as

$$\dot{g} = [g, H + u_m\phi_m]\,. \tag{1-16}$$

Here you see the coefficients u occurring in one of the members of a Poisson bracket. The coefficients u_m are not functions of the q 's and the p 's, so that we cannot use the definition (1-9) for determining the Poisson bracket in (1-16). However, we can proceed to work out

this Poisson bracket using the laws (1-10), (1-11), (1-12), and (1-13). Using the summation law (1-11) we have:

$$[g, H + u_m\phi_m] = [g, H] + [g, u_m\phi_m] \tag{1-17}$$

and using the product law (1-12),

$$[g, u_m\phi_m] = [g, u_m]\,\phi_m + u_m\,[g, \phi_m] \tag{1-18}$$

The last bracket in (1-18) is well-defined, for g and ϕ_m are both functions of the q 's and the p 's. The Poisson bracket $[\ g, u_m\ ]$ is not defined, but it is multiplied by something that vanishes, ϕ_m. So the first term on the right of (1-18) vanishes. The result is that

$$[g, H + u_m\phi_m] = [g, H] + u_m [g, \phi_m] \tag{1-19}$$

making (1-16) agree with (1-15).

There is something that we have to be careful about in working with the Poisson bracket formalism: We have the constraints (1-4), but must not use one of these constraints before working out a Poisson bracket. If we did, we would get a wrong result. So we take it as a rule that Poisson brackets must all be worked out before we make use of the constraint equations. To remind us of this rule in the formalism, I write the constraints (1-4) as equations with a different equality sign $\approx$ from the usual. Thus they are written

$$\phi_m \approx 0. \tag{1-20}$$

I call such equations weak equations, to distinguish them from the usual or strong equations.

One can make use of (1-20) only after one has worked out all the Poisson brackets which one is interested in. Subject to this rule, the Poisson bracket (1-19) is quite

definite, and we have the possibility of writing our cquations of motion (1-16) in a very concise form:

$$\dot{g} \approx [g, H_T] \tag{1-21}$$

with a Hamiltonian I call the total Hamiltonian,

$$H_T = H + u_m\phi_m. \tag{1-22}$$

Now let us examine the consequences of these cquations of motion. In the first place, there will be some consistency conditions. We have the quantities ϕ which have to be zero throughout all time. We can apply the equation of motion (1-21) or (1-15) taking g to be one of the ϕ 's. We know that $\dot{g}$ must be zero for consistency, and so we get some consistency conditions. Let us see what they are like. Putting $g = \phi_m$ and $\dot{g} = 0$ in (1-15), we have:

$$[\phi_m, H] + u_{m'} [\phi_m, \phi_{m'}] \approx 0 \tag{1-23}$$

We have here a number of consistency conditions, one for each value of m. We must examine these conditions to see what they lead to. It is possible for them to lead directly to an inconsistency. They might lead to the inconsistency $1 = 0$. If that happens, it would mean that our original Lagrangian is such that the Lagrangian equations of motion are inconsistent. One can easily construct an example with just one degree of freedom. If we take $L = q$ then the Lagrangian equation of motion (1-2) gives immediately $1 = 0$. So you see, we cannot take the Lagrangian to be completely arbitrary. We must impose on it the condition that the Lagrangian equations of motion do not involve an inconsistency. With this restriction the equations (1-23) can be divided into three kinds.

One kind of equation reduces to $0 = 0$, i.e. it is identically satisfied, with the help of the primary constraints.

Another kind of equation reduces to an equation independent of the u 's, thus involving only the q 's and the p 's. Such an equation must be independent of the primary constraints, otherwise it is of the first kind. Thus it is of the form

$$\chi(q, p) = 0. \tag{1-24}$$

Finally, an equation in (1-23) may not reduce in either of these ways; it then imposes a condition on the u 's.

The first kind we do not have to bother about any more. Each equation of the second kind means that we have another constraint on the Hamiltonian variables. Constraints which turn up in this way are called secondary constraints. They differ from the primary constraints in that the primary constraints are consequences merely of the equations (1-3) that define the momentum variables, while for the secondary constraints, one has to make use of the Lagrangian equations of motion as well.

If we have a secondary constraint turning up in our theory, then we get yet another consistency condition, because we can work out $\dot{\chi}$ according to the equation of motion (1-15) and we require that $\dot{\chi} \approx 0$. So we get another equation

$$[\chi, H] + u_m [\chi, \phi_m] \approx 0. \tag{1-25}$$

This equation has to be treated on the same footing as (1-23). One must again see which of the three kinds it is. If it is of the second kind, then we have to push the process one stage further because we have a further

[14]

wondary constraint. We carry on like that until we have whausted all the consistency conditions, and the final wsult will be that we are left with a number of secondary constraints of the type (1-24) together with a number of conditions on the coefficients u of the type (1-23).

The secondary constraints will for many purposes be licated on the same footing as the primary constraints. It is convenient to use the notation for them:

$$\phi_k \approx 0, \quad k = M + 1, ..., M + K \tag{1-26}$$

where K is the total number of secondary constraints. They ought to be written as weak equations in the same way as primary constraints, as they are also equations which one must not make use of before one works out Poisson brackets. So all the constraints together may be written as

$$\phi_j \approx 0, \quad j = 1, ..., M + K \equiv \mathscr{F}. \tag{1-27}$$

Let us now go over to the remaining equations of the third kind. We have to see what conditions they impose on the coefficients u. These equations are

$$[\phi_j, H] + u_m [\phi_j, \phi_m] \approx 0 \tag{1-28}$$

where m is summed from 1 to M and j takes on any of the values from 1 to 7 . We have these equations involving conditions on the coefficients u, insofar as they do not reduce merely to the constraint equations.

Let us look at these equations from the following point of view. Let us suppose that the u 's are unknowns and that we have in (1-28) a number of non-homogeneous linear equations in these unknowns u, with coefficients which are functions of the q 's and the p 's. Let us look

[15]

for a solution of these equations, which gives us the u 's as functions of the q 's and the p 's, say

$$u_m = U_m(q, p) \tag{1-29}$$

There must exist a solution of this type, because if there were none it would mean that the Lagrangian equations of motion are inconsistent, and we are excluding that case.

The solution is not unique. If we have one solution, we may add to it any solution $V_m(q,p)$ of the homogeneous equations associated with (1-28):

$$V_m\left[\phi_j, \phi_m\right] = 0 \tag{1-30}$$

and that will give us another solution of the inhomogeneous equations (1-28). We want the most general solution of (1-28) and that means that we must consider all the independent solutions of (1-30), which we may denote by $V_{am}(q,p), a = 1, ..., A$. The general solution of (1-28) is then

$$u_m = U_m + v_a V_{am}, \tag{1-31}$$

in terms of coefficients v_a which can be arbitrary.
Let us substitute these expressions for u into the total Hamiltonian of the theory (1-22). That will give us the total Hamiltonian

$$H_T = H + U_m\phi_m + v_a V_{am}\phi_m \tag{1-32}$$

We can write this as

$$H_T = H' + v_a\phi_a, \tag{1-33}$$

where

$$H' = H + U_m\phi_m \tag{1-33}$$

and

$$\phi_a = V_{am}\phi_m. \tag{1-34}$$

In terms of this total Hamiltonian (1-33) we still have the equations of motion (1-21).

As a result of carrying out this analysis, we have ratisfied all the consistency requirements of the theory and we still have arbitrary coefficients v. The number of the coefficients v will usually be less than the number of coefficients u. The u 's are not arbitrary but have to atisfy consistency conditions, while the v's are arbitrary coefficients. We may take the v's to be arbitrary functions of the time and we have still satisfied all the requirements of our dynamical theory.

This provides a difference of the generalized Hamilonnian formalism from what one is familiar with in clementary dynamics. We have arbitrary functions of the time occurring in the general solution of the equations of motion with given initial conditions. These arbitrary lunctions of the time must mean that we are using a mathematical framework containing arbitrary features, for example, a coordinate system which we can choose in some arbitrary way, or the gauge in electrodynamics. As a result of this arbitrariness in the mathematical framework, the dynamical variables at future times are not completely determined by the initial dynamical variables, and this shows itself up through arbitrary functions appearing in the general solution.

We require some terminology which will enable one to appreciate the relationships between the quantities which occur in the formalism. I find the following terminology useful. I define any dynamical variable, R, a function of the q 's and the p 's, to be first-class if it has zero Poisson brackets with all the ϕ 's:

$$[R, \phi_j] \approx 0, \quad j = 1, ..., \mathscr{F} \tag{1-35}$$

[17]

It is sufficient if these conditions hold weakly. Otherwise R is second-class. If R is first-class, then $[R, \phi_j]$ has to be strongly equal to some linear function of the ϕ 's, as anything that is weakly zero in the present theory is strongly equal to some linear function of the ϕ 's. The ϕ 's are, by definition, the only independent quantities which are weakly zero. So we have the strong equations

$$[R, \phi_j] = r_{jj'}\phi_{j'}. \tag{1-36}$$

Before going on, I would like to prove a
Theorem: the Poisson bracket of two first-class quantities is also first-class. Proof. Let R, S be first-class: then in addition to (1-36), we have

$$[S, \phi_j] = s_{jj'}\phi_{j'} \tag{1-36}$$

Let us form $[[R, S], \phi_j]$. We can work out this Poisson bracket using Jacobi's identity (1-13)

$$\begin{aligned}
[[R, S], \phi_j] &= [[R, \phi_j], S] - [[S, \phi_j], R] \\
&= [r_{jj'}\phi_{j'}, S] - [s_{jj'}\phi_{j'}, R] \\
&= r_{jj'}[\phi_{j'}, S] + [r_{jj'}, S]\phi_{j'} - s_{jj'}[\phi_{j'}, R] \\
&- [s_{jj'}, R]\phi_{j'} \\
&\approx 0
\end{aligned}$$

by (1-36), (1-36)', the product law (1-12), and (1-20). The whole thing vanishes weakly. We have proved therefore that $[R, S]$ is first-class.

We have altogether four different kinds of constraints. We can divide constraints into first-class and secondclass, which is quite independent of the division into primary and secondary.

I would like you to notice that H' given by $(1-33)'$ and

thr ϕ_a given by (1-34) are first-class. Forming the Prisson bracket of ϕ_a with ϕ_j we get, by (1-34), $_{1\ldots}||_m, \phi_j]$ plus terms that vanish weakly. Since the I_{4m} are defined to satisfy ($1-30$), ϕ_a is first-class. immilarly (1-28) with U_m for u_m shows that H' is first– lass. Thus (1-33) gives the total Hamiltonian in terms . 11 a first-class Hamiltonian H' together with some first– hass ϕ 's.

Any linear combination of the ϕ 's is of course another constraint, and if we take a linear combination of the primary constraints we get another primary constraint. io each ϕ_a is a primary constraint; and it is first-class. So the final situation is that we have the total Hamiltomian expressed as the sum of a first-class Hamiltonian plus a linear combination of the primary, first-class constraints.

The number of independent arbitrary functions of the tume occurring in the general solution of the equations of motion is equal to the number of values which the suffix a takes on. That is equal to the number of independent primary first-class constraints, because all the independcut primary first-class constraints are included in the sum (1-33).

That gives you then the general situation. We have deduced it by just starting from the Lagrangian equations of motion, passing to the Hamiltonian and working out consistency conditions.

From the practical point of view one can tell from the general transformation properties of the action integral what arbitrary functions of the time will occur in the general solution of the equations of motion. To each of these functions of the time there must correspond some primary first-class constraint. So we can tell which

primary first-class constraints we are going to have without going through all the detailed calculation of working out Poisson brackets; in practical applications of this theory we can obviously save a lot of work by using that method.

I would like to go on a bit more and develop one further point of the theory. Let us try to get a physical understanding of the situation where we start with given initial variables and get a solution of the equations of motion containing arbitrary functions. The initial variables which we need are the q 's and the p 's. We don't need to be given initial values for the coefficients v. These initial conditions describe what physicists would call the initial physical state of the system. The physical state is determined only by the q 's and the p 's and not by the coefficients τ.

Now the initial state must determine the state at later times. But the q 's and the p 's at later times are not uniquely determined by the initial state because we have the arbitrary functions v coming in. That means that the state does not uniquely determine a set of q 's and p 's, even though a set of q 's and p 's uniquely determines a state. There must be several choices of q 's and p 's which correspond to the same state. So we have the problem of looking for all the sets of q 's and p 's that correspond to one particular physical state.

All those values for the q 's and p 's at a certain time which can evolve from one initial state must correspond to the same physical state at that time. Let us take particular initial values for the q 's and the p 's at time $t = 0$, and consider what the q 's and the p 's are after a short time interval δt. For a general dynamical variable g, with initial value g_0, its value at time δt is

$$\begin{aligned} g(\delta t) &= g_0 + \dot{g}\delta t \\ &= g_0 + [g, H_T]\,\delta t \\ &= g_0 + \delta t\,\{[g, H'] + v_a\,[g, \phi_a]\}\,. \end{aligned} \tag{1-37}$$

The coefficients v are completely arbitrary and at our disposal. Suppose we take different values, v', for these coefficients. That would give a different $g(\delta t)$, the difference being

$$\Delta g(\delta t) = \delta t\,(v_a - v'_a)\,[g, \phi_a] \tag{1-38}$$

We may write this as

$$\begin{aligned} &\Delta g(\delta t) = \varepsilon_a\,[g, \phi_a]\,, \\ \text{where}\quad &\varepsilon_a = \delta t\,(v_a - v'_a) \end{aligned}$$

is a small arbitrary number, small because of the coefficient δt and arbitrary because the v 's and the v 's are arbitrary. We can change all our Hamiltonian variables in accordance with the rule (1-39) and the new Hamiltonian variables will describe the same state. This change in the Hamiltonian variables consists in applying an infinitesimal contact transformation with a generating function $\varepsilon_a\phi_a$. We come to the conclusion that the ϕ_a 's, which appeared in the theory in the first place as the primary first-class constraints, have this meaning: as generating functions of infinitesimal contact transformations, they lead to changes in the q's and the p's that do not affect the physical state.

However, that is not the end of the story. We can go on further in the same direction. Suppose we apply two of these contact transformations in succession. Apply first a contact transformation with generating function

$\varepsilon_a\phi_a$ and then apply a second contact transformation with generating function $\gamma_{a'}\phi_{a'}$, where the gamma's are some new small coefficients. We get finally

$$g' = g_0 + \varepsilon_a [g, \phi_a] + \gamma_{a'} [g + \varepsilon_a [g, \phi_a], \phi_{a'}] . (1 - 41)$$

(I retain the second order terms involving products $\varepsilon\gamma$, but I neglect the second order terms involving ε^2 or involving γ^2. This is legitimate and sufficient. I do that because I do not want to write down more than I really need for getting the desired result.) If we apply the two transformations in succession in the reverse order, w get finally

$$g'' = g_0 + \gamma_{a'} [g, \phi_{a'}] + \varepsilon_a [g + \gamma_{a'} [g, \phi_{a'}], \phi_a] . \quad (1\text{-}42)$$

Now let us subtract these two. The difference is

$$\Delta g = \varepsilon_a \gamma_{a'} \{[[g, \phi_a], \phi_{a'}] - [[g, \phi_{a'}], \phi_a]\} . \quad (1\text{-}43)$$

By Jacobi's identity (1-13) this reduces to

$$\Delta g = \varepsilon_a \gamma_{a'} [g, [\phi_a, \phi_{a'}]] . \quad (1\text{-}44)$$

This Δg must also correspond to a change in the q 's and the p 's which does not involve any change in the physical state, because it is made up by processes which individually don't involve any change in the physical state. Thus we see that we can use

$$[\phi_a, \phi_{a'}] \quad (1\text{-}45)$$

as a generating function of an infinitesimal contact transformation and it will still cause no change in the physical state.

Now the ϕ_a are first-class: their Poisson brackets are walkly zero, and therefore strongly equal to some linear function of the ϕ 's. This linear function of the ϕ 's must low lirst-class because of the theorem I proved a little while back, that the Poisson bracket of two first-class quantities is first-class. So we see that the transformations which we get this way, corresponding to no change in the physical state, are transformations for which the generalong function is a first-class constraint. The only way these transformations are more general than the ones we had before is that the generating functions which we had before are restricted to be first-class primary constraints. Those that we get now could be first-class secondary constraints. The result of this calculation is to show that we might have a first-class secondary constraint as a penerating function of an infinitesimal contact translormation which leads to a change in the q 's and the p 's without changing the state.

For the sake of completeness, there is a little bit of lurther work one ought to do which shows that a Poisson bracket [H', ϕ_a] of the first-class Hamiltonian H' with a first-class ϕ is again a linear function of first-class constraints. This can also be shown to be a possible generator for infinitesimal contact transformations which do not change the state.

The final result is that those transformations of the dynamical variables which do not change physical states are infinitesimal contact transformations in which the generating function is a primary first-class constraint or possibly a secondary first-class constraint. A good many of the secondary first-class constraints do turn up by the process (1-45) or as [H', ϕ_a]. I think it may be that all the first-class secondary constraints should be included

among the transformations which don't change the physical state, but I haven't been able to prove it. Also, I haven't found any example for which there exist first-class secondary constraints which do generate a change in the physical state.

24.5.3 Dirac's Lecture 2: The Problem of Quantization

We were led to the idea that there are certain changes in the p 's and q 's that do not correspond to a change of tate, and which have as generators first-class secondary constraints. That suggests that one should generalize the rquations of motion in order to allow as variation of a dynamical variable g with the time not only any variation piven by (1-21), but also any variation which does not correspond to a change of state. So we should consider a more general equation of motion

$$\dot{g} = [g, H_E] \tag{2-1}$$

with an extended Hamiltonian H_E, consisting of the previous Hamiltonian, H_T, plus all those generators which do not change the state, with arbitrary coefficients:

$$H_E = H_T + v'_{a'}\phi_{a'} \tag{2-2}$$

'l'hose generators $\phi_{a'}$, which are not included already in H_T will be the first-class secondary constraints. The presence of these further terms in the Hamiltonian will give further changes in g, but these further changes in g do not correspond to any change of state and so they should certainly be included, even though we did not

arrive at these further changes of g by direct work from the Lagrangian.

That, then, is the general Hamiltonian theory. The theory as I have developed it applies to a finite number of degrees of freedom but we can easily extend it to the case of an infinite number of degrees of freedom. Our suffix denoting the degree of freedom is $n = 1, ..., N$; we may easily make N infinite. We may further generalize it by allowing the number of degrees of freedom to be continuously infinite. That is to say, we may have as our q 's and p 's variables q_x, p_x where x is a suffix which can take on all values in a continuous range. If we work with this continuous x, then we have to change all our sums over n in the previous work into integrals. The previous work can all be taken over directly with this change.

There is just one equation which we will have to think of a bit differently, the equation which defines the momentum variables,

$$p_n = \frac{dL}{d\dot{q}_n}. \tag{1-3}$$

If n takes on a continuous range of values, we have to understand by this partial differentiation a process of partial functional differentiation that can be made precise in this way: We vary the velocities by $\delta\dot{q}_x$ in the Lagrangian and then put

$$\delta L = \int p_x \delta\dot{q}_x \tag{2-3}$$

The coefficient of $\delta\dot{q}_x$ occurring in the integrand in δL is defined to be p_x.

After giving this general abstract theory, I think it would be a help if I gave a simple example as illustration.

I will take as an example just the electromagnetic field of Maxwell, which is defined in terms of potentials A_μ. The dynamical coordinates now consist of the potentials tor all points of space at a certain time. That is to say, the dynamical coordinates consist of $A_{\mu x}$, where the suffix x a ands for the three coordinates x^1, x^2, x^3 of a point in three-dimensional space at a certain time x^0 (not the lour x 's which one is used to in relativity). We shall have then as the dynamical velocities the time derivatives of the dynamical coordinates, and I shall denote these by a nuffix 0 preceded by a comma.

Any suffix with a comma before it denotes differentiaton according to the general scheme

$$\xi_{,\mu} = \frac{d\xi}{dx^\mu} \tag{2-4}$$

We are dealing with special relativity so that we can raise and lower these suffixes according to the rules of upecial relativity: we have a change in sign if we raise or lower a suffix 1,2 , or 3 but no change of sign when we taise or lower the suffix 0 .

We have as our Lagrangian for the Maxwell electrodynamics, if we work in Heaviside units,

$$L = -\frac{1}{4}\int F_{\mu v}F^{\mu y}d^3x \tag{2-5}$$

Here d^3x means $dx^1dx^2dx^3$, the integration is over three-dimensional space, and $F_{\mu\nu}$ means the field quantities defined in terms of the potentials by

$$F_{\mu v} = A_{v,\mu} - A_{\mu,v}. \tag{2-6}$$

This L is the Lagrangian because its time integral is the action integral of the Maxwell field.

Let us now take this Lagrangian and apply the rules of our formalism for passing to the Hamiltonian. We first of all have to introduce the momenta. We do that by varying the velocities in the Lagrangian. If we vary the velocities, we have

$$\begin{aligned}\delta L &= -\frac{1}{2}\int F^{\mu v}\delta F_{\mu v}d^3x \\ &= \int F^{\mu 0}\delta A_{\mu,0}d^3x\end{aligned} \tag{2-7}$$

Now the momenta B^μ are defined by

$$\delta L = \int B^\mu \delta A_{\mu 0}d^3x \tag{2-8}$$

and these momenta will satisfy the basic Poisson bracket relations

$$[A_{ux}, B^v_{x'}] = g^v_\mu \delta^3(x - x')\,; \quad \mu, \nu = 0, 1, 2, 3. \tag{2-9}$$

In this formula A is taken at a point x in three-dimensional space and B is taken at a point x' in the threedimensional space. g^ν_μ is just the Kronecker delta function. $\delta^3(x - x')$ is the three-dimensional delta function of $x - x'$.

We compare the two expressions (2-7) and (2-8) for δL and that gives us

$$B^\mu = F^{\mu 0} \tag{2-10}$$

Now $F^{\mu v}$ is anti-symmetrical

$$F^{\mu v} = -F^{\nu\mu} \tag{2-11}$$

So if we put $\mu = 0$, in (2-10) we get zero. Thus B^0_x is
equal to zero. This is a primary constraint. I write it as a weak equation:

$$B^0_x \approx 0 \tag{2-12}$$

The other three momenta $B^r (r = 1, 2, 3)$ are just equal to the components of the electric field.

I should remind you that (2-12) is not just one primary constraint: there is a whole threefold infinity of primary constraints because there is the suffix x which stands for some point in three-dimensional space; and each value for x will give us a different primary constraint.

Let us now introduce the Hamiltonian. We define that in the usual way by

$$\begin{aligned} H &= \int B^{\mu} A_{\mu,0} d^3x - L \\ &= \int \left(F^{r0} A_{r,0} + \frac{1}{4} F^{rs} F_{rs} + \frac{1}{2} F^{r0} F_{r0} \right) d^3x \\ &= \int \left(\frac{1}{4} F^{rs} F_{rs} - \frac{1}{2} F^{r0} F_{r0} + F^{r0} A_{0,r} \right) d^3x \\ &= \int \left(\frac{1}{4} F^{rs} F_{rs} + \frac{1}{2} B^r B^r - A_0 B^r_{\ r} \right) d^3x \end{aligned} \tag{2-13}$$

I've done a partial integration of the last term in (2-13) to get it in this form. Now here we have an expression for the Hamiltonian which does not involve any velocities. It involves only dynamical coordinates and momenta. It is true that F_{rs} involves partial differentiations of the potentials, but it involves partial differentiations only with respect to x^1, x^2, x^3. That does not bring in any velocities. These partial derivatives are functions of the dynamical coordinates.

We can now work out the consistency conditions by

using the primary constraints (2-12). Since they have to remain satisfied at all times, $[B^0, H]$ has to be zero. This leads to the equation

$$B^r_{\ ,r} \approx 0 \tag{2-14}$$

This is again a constraint because there are no velocities occurring in it. This is a secondary constraint, which appears in the Maxwell theory in this way. If we proceed further to examine the consistency relations, we must work out

$$\left[B^r_{\ ,r}, H \right] = 0 \tag{2-15}$$

We find that this reduces to $0 = 0$. It does not give us anything new, but is automatically satisfied. We have therefore obtained all the constraints in our problem. (2-12) gives the primary constraints. (2-14) gives the secondary constraints.

We now have to look to see whether they are first-class or second-class, and we easily see that they are all firstclass. The B_0 are momenta variables. They all have zero Poisson brackets with each other. $B^r_{\ ,r}$ and B_0 also have zero Poisson brackets with each other. And B^r_{rx} and $B^r_{r,x'}$ also have zero Poisson brackets with cach other. All these quantities are therefore first-class constraints. There are no second-class constraints occurring in the Maxwell electrodynamics.

The expression (2-13) for H is first-class, so this H can be taken as the H' of (1-33). Let us now see what the total Hamiltonian is:

$$\begin{aligned} H_T = \int \left(\frac{1}{4} F^{rs} F_{rs} + \frac{1}{2} B_r B_r \right) d^3x - \int A_0 B^r_{\ ,r} d^3x \\ + \int v_x B^0 d^3x \end{aligned} \tag{2-16}$$

[30]

This v_x is an arbitrary coefficient for each point in threedimensional space. We have just added on the primary first-class constraints with arbitrary coefficients, which is what we must do according to the rules to get the total Hamiltonian.

In terms of the total Hamiltonian we have the equation of motion in the standard form

$$\dot{g} \approx [g, H_T] \tag{1-21}$$

The g which we have here may be any field quantity at some point x in three-dimensional space, or may also be a function of field quantities at different points in threedimensional space. It could, for example, be an integral over three-dimensional space. This g can be perfectly generally any function of the q 's and the p 's throughout three-dimensional space.

It is permissible to take $g = A_0$ and then we get

$$A_{0,0} = v \tag{2-17}$$

because A_0 has zero Poisson brackets with everything except the B_0 occurring in the last term of (2-16). This gives us a meaning for the arbitrary coefficient v_x occurring in the total Hamiltonian. It is the time derivative of A_0.

Now to get the most general motion which is physically permissible, we ought to pass over to the extended llamiltonian. To do this we add on the first-class mecondary constraints with arbitrary coefficients u_x. This gives the extended Hamiltonian:

$$H_E = H_T + \int u_x B^r_{,r} d^3x \tag{2-18}$$

Bringing in this extra term into the Hamiltonian allows

a more general motion. It gives more variation of the q 's and the p 's, of the nature of a gauge transformation. When this additional variation of the q 's and the p 's is brought in, it leads to a further set of q 's and p 's which must correspond to the same state.

That is the result of working out, according to our rules, the Hamiltonian form of the Maxwell theory. When we've got to this stage, we see that there is a certain simplification which is possible. This simplification comes about because the variables A_0, B_0 are not of any physical significance. Let us see what the equations of motion tell us about A_0 and B_0.$B_0 = 0$ all the time. That is not of interest. A_0 is something whose time derivative is quite arbitrary. That again is something which is not of interest. The variables A_0 and B_0 are therefore not of interest at all. We can drop them out from the theory and that will lead to a simplified Hamiltonian formalism where we have fewer degrees of freedom, but still retain all the degrees of freedom which are physically of interest.

In order to carry out this discard of the variables A_0 and B_0, we drop out the term $v_x B^0$ from the Hamiltonian. This term merely has the effect of allowing A_0 to vary arbitrarily. The term - $A_0 B^r_{,r}$ in H_T can be combined with the $u_x B^r_{,r}$ in the extended Hamiltonian. The coefficient u_x is an arbitrary coefficient in any case. When we combine these two terms, we just have this u_x replaced by $u'_x = u_x - A_0$ which is equally arbitrary. So that we get a new Hamiltonian

$$H = \int \left(\frac{1}{4} F^{rs} F_{rs} + \frac{1}{2} B_r B_r \right) d^3x + \int u'_x B^r_{,r} d^3x \tag{2-19}$$

This Hamiltonian is sufficient to give the equations of motion for all the variables which are of physical interest. The variables A_0, B_0 no longer appear in it. This is the Hamiltonian for the Maxwell theory in its simplest form.

Now the usual Hamiltonian which people work with in quantum electrodynamics is not quite the same as that. The usual one is based on a theory which was originally set up by Fermi. Fermi's theory involves putting this restriction on the potentials:

$$A^\mu_{,\mu} = 0. \tag{2-20}$$

It is quite permissible to bring in this restriction on the gauge. The Hamiltonian theory which I have given here does not involve this restriction, so that it allows a completely general gauge. It's thus a somewhat different formalism from the Fermi formalism. It's a formalism which displays the full transforming power of the Maxwell theory, which we get when we have

completely general changes of gauge. This Maxwell theory gives us an illustration of the general ideas of primary and "condary constraints.

I would like now to go back to general theory and to consider the problem of quantizing the Hamiltonian theory. To discuss this question of quantization, let us lirst take the case when there are no second-class constraints, when all the constraints are first-class. We make our dynamical coordinates and momenta, the q 's ...nd p 's, into operators satisfying commutation relations which correspond to the Poisson bracket relations of the classical theory. That is quite straightforward. Then we ut up a Schrödinger equation

$$i\hbar\frac{d\psi}{dt} = H'\psi. \tag{2-21}$$

ψ is the wave function on which the q 's and the p 's operate. H' is the first-class Hamiltonian of our theory.

We further impose certain supplementary conditions on the wave function, namely:

$$\phi_j\psi = 0 \tag{2-22}$$

Each of our constraints thus leads to a supplementary condition on the wave function. (The constraints, remember, are now all first-class.)

The first thing we have to do now is to see whether these equations for ψ are consistent with one another. Let us take two of the supplementary conditions and see whether they are consistent. Let us take (2-22) and

$$\phi_{j'}\psi = 0 \tag{2-22}$$

If we multiply (2-22) by $\phi_{j'}$, we get

$$\phi_{j'}\phi_j\psi = 0 \tag{2-23}$$

If we multiply $(2-22)'$ by ϕ_j, we get

$$\phi_j\phi_{j'}\psi = 0. \tag{2-23}$$

If we now subtract these two equations, we get:

$$[\phi_j, \phi_{j'}]\,\psi = 0 \tag{2-24}$$

This further condition on ψ is necessary for consistency. Now we don't want to have any fresh conditions on ψ. We want all the conditions on ψ to be included among (2-22). That means to say, we want to have (2-24) a consequence of (2-22) which means we require

$$[\phi_j, \phi_{j'}] = c_{jj'j''}\phi_{j''}. \tag{2-25}$$

[34]

If (2-25) does hold, then (2-24) is a consequence of (2-22) and is not a new condition on the wave function.

Now we know that the ϕ 's are all first-class in the classical theory, and that means that the Poisson bracket of any two of the ϕ 's is a linear combination of the ϕ 's in the classical theory. When we go over to the quantum theory, we must have a similar equation holding for the commutator, but it does not necessarily follow that the coefficients c are all on the left. We need to have these coefficients all on the left, because the c 's will in general be functions of the coordinates and momenta and will not commute with the ϕ 's in the quantum theory, and (2-24) will be a consequence of (2-22) only provided the c's are all on the left.

When we set up the quantities ϕ in the quantum theory, there may be some arbitrariness coming in. The corresponding classical expressions may involve quantities which don't commute in the quantum theory and then we have to decide on the order in which to put the lactors in the quantum theory. We have to try to arrange the order of these factors so that we have (2-25) holding with all the coefficients on the left. If we can do that, then we have the supplementary conditions all consistent with each other. If we cannot do it, then we are out of luck and we cannot make an accurate quantum theory. In any case we have a first approximation to the quantum theory, because our equations would be all right if we look at them only to the order of accuracy of Planck's constant $\hbar$ and neglect quantities of order $\hbar^2$.

I have just discussed the requirements for the supplementary conditions to be consistent with one another. There is a similar discussion needed in order to check that the supplementary conditions shall be consistent

with the Schrödinger equation. If we start with a ψ satisfying the supplementary conditions (2-24) and let that ψ vary with the time in accordance with the Schrödinger equation, then after a lapse of a short interval of time will our ψ still satisfy the supplementary conditions? We can work out the requirement for that to be the case and we get

$$[\phi_j, H]\,\psi = 0 \tag{2-26}$$

which means that $[\phi_j, H]$ must be some linear function of the ϕ 's :

$$[\phi_j, H] = b_{jj'}\phi_{j'} \tag{2-27}$$

if we are not to get a new supplementary condition. Again we have an equation which we know is all right in the classical theory. ϕ_j and H are both first-class, so their Poisson bracket vanishes weakly. The Poisson bracket is thus strongly equal to some linear function of the ϕ 's in the classical theory. Again we have to try to arrange things so that in the corresponding quantum equation we have all our coefficients on the left. That is necessary to get an accurate quantum theory, and we need a bit of luck, in general, in order to be able to bring it about.

Let us now consider how to quantize a Hamiltonian theory in which there are second-class constraints. Let us think of this question first in terms of a simple example. We might take as the simplest example of two second-class constraints

$$q_1 \approx 0 \text{ and } p_1 \approx 0 \tag{2-28}$$

If we have these two constraints appearing in the theory, then their Poisson bracket is not zero, so they

are second-class. What can we do with them when we go over to the quantum theory? We cannot impose (2-28) as supplementary conditions on the wave function as we did with the first-class constraints. If we try to put $q_1\psi = 0, p_1\psi = 0$, then we should immediately get a contradiction because we should have $(q_1p_1 - p_1q_1)\,\psi = i\hbar\psi = 0$. So that won't do. We must adopt some different plan.

Now in this simple case it's pretty obvious what the plan must be. The variables q_1 and p_1 are not of interest if they are both restricted to be zero. So the degree of freedom 1 is not of any importance. We can just discard the degree of freedom 1 and work with the other degrees of freedom. That means a different definition for a Poisson bracket. We should have to work with a definition of a Poisson bracket in the classical theory

$$[\xi, \eta] = \frac{\partial\xi}{\partial q_n}\frac{\partial\eta}{\partial p_n} - \frac{\partial\xi}{\partial p_n}\frac{\partial\eta}{\partial q_n} \quad \text{summed over } n = 2, \ldots N. \tag{2-29}$$

This would be sufficient because it would deal with all the variables which are of physical interest. Then we could just take q_1 and p_1 as identically zero. There's no contradiction involved

there, and we can pass over to the quantum theory, setting it up in terms only of the degrees of freedom $n = 2, ..., N$.

In this simple case it is fairly obvious what we have to do to build up a quantum theory. Let us try now to generalize it. Suppose we have $p_1 \approx 0, q_1 \approx f(q_r, p_r)$, $r = 2, ..., N$, so f is any function of all the other q 's and p 's. We could drop out the number 1 degree of freedom if we substitute $f(q_r, p_r)$ for q_1 in the Hamiltonian and in all the other constraints. Again we can forget

about the number 1 degree of freedom and simply work with the other degrees of freedom and pass over to a quantum theory in these other degrees of freedom. Again we should have to work with the (2-29) kind of Poisson bracket, referring only to the other degrees of freedom.

That is the idea which one uses for quantizing a theory which involves second-class constraints. The existence of second-class constraints means that there are some degrees of freedom which are not physically important. We have to pick out these degrees of freedom and set up new Poisson brackets referring only to the other degrees of freedom which are of physical importance. Then in terms of those new Poisson brackets we can pass over to the quantum theory. I would like to discuss a general procedure for carrying that out.

For the present, we are going back to the classical theory. We have a number of constraints $\phi_j \approx 0$, some of them first-class, some second-class. We can replace these constraints by independent linear combinations of them, which will do just as well as the original constraints. We try to arrange to take the linear combinations in such a way as to have as many constraints as possible brought into the first class. There may then be some left in the second class which we just cannot bring into the first class by taking linear combinations of them. Those which are left in the second class I will call χ_s, $s = 1, ..., S$ is the number of second-class constraints which are such that no linear combination of them is first-class.

We take these surviving second-class constraints and we form all their Poisson brackets with each other and arrange these Poisson brackets as a determinant Δ :

THE PROBLEM OF QUANTIZATION

$$\Delta = \begin{vmatrix} 0 & [\chi_1, \chi_2] & [\chi_1, \chi_3] & \cdots & [\chi_1, \chi_S] \\ [\chi_2, \chi_1] & 0 & [\chi_2, \chi_3] & \cdots & [\chi_2, \chi_S] \\ \vdots & \vdots & \vdots & & \vdots \\ [\chi_S, \chi_1] & [\chi_S, \chi_2] & [\chi_S, \chi_3] & \cdots & \vdots \end{vmatrix}$$

I would like now to prove a

Theorem: The determinant Δ does not vanish, not even weakly. Proof: Assume that the determinant does vanish. I'm going to show that we get a contradiction. If the determinant vanishes, then it is of some rank $T < S$. Now let us set up the determinant A :

$$A = \begin{vmatrix} \chi_1 & 0 & [\chi_1, \chi_2] & \cdots & [\chi_1, \chi_T] \\ \chi_2 & [\chi_2, \chi_1] & 0 & & [\chi_2, \chi_T] \\ \vdots & \vdots & \vdots & & \vdots \\ \chi_{T+1} & [\chi_{T+1}, \chi_1] & [\chi_{T+1}, \chi_2] & \cdots & [\chi_{T+1}, \chi_T] \end{vmatrix}$$

1 has $T + 1$ rows and columns. $T + 1$ might equal S or might be less than S. If we expand A in terms of the clements of its first column, we will get each of these dements multiplied into one of the sub-determinants of 1. Now I don't want all of these sub-determinants to vanish. It might so happen that they do all vanish. And in that case, I would choose the χ 's which are referred to mong the rows and columns of A in a different way. There must always be some way of choosing the χ 's which occur in A so that the sub-determinants don't all valuish, because Δ is of rank T. So we choose the χ 's in auch a way that the coefficients of the elements in the first column are not all zero.

Now I will show that A has zero Poisson brackets with ....y of the ϕ 's. If we form the Poisson bracket of ϕ with 'determinant, we get the result by forming the Poisson bracket of ϕ with the first column of the determinant, adding on the result of forming the Poisson bracket of ϕ with the second column of the determinant, and so on. Thus

$$
\begin{aligned}
[\phi, A] = &\begin{vmatrix} [\phi,\chi_1] & 0 & \cdots \\ [\phi,\chi_2] & [\chi_2,\chi_1] & \cdots \\ \vdots & \vdots & \\ [\phi,\chi_{T+1}] & [\chi_{T+1},\chi_1] & \cdots \end{vmatrix} \\
&+ \begin{vmatrix} \chi_1 & 0 & \cdots \\ \chi_2 & [\phi,[\chi_2,\chi_1]] & \cdots \\ \vdots & \vdots & \\ \chi_{T+1} & [\phi,[\chi_{T+1},\chi_1]] & \cdots \end{vmatrix} \\
&+ \begin{vmatrix} \chi_1 & 0 & [\phi,[\chi_1,\chi_2]] & \cdots \\ \chi_2 & [\chi_2,\chi_1] & 0 & \cdots \\ \vdots & \vdots & \vdots & \\ \chi_{T+1} & [\chi_{T+1},\chi_1] & [\phi,[\chi_{T+1},\chi_2]] & \cdots \end{vmatrix} + \cdots
\end{aligned}
$$

This looks rather complicated, but one can easily see that every one of these determinants vanishes. In the first place, the first determinant on the right vanishes: if ϕ is first class, then the first column vanishes; if ϕ is second class, then ϕ is one of the χ 's and we have a determinant which is a part of the determinant Δ with $T+1$ rows and columns. But Δ is assumed to be of rank T, so that any part of it with $T+1$ rows and columns vanishes. Now, the second determinant on the right vanishes weakly because the first column vanishes weakly. Similarly all the other determinants vanish weakly. The result is that the whole right-hand side vanishes weakly.

Thus A is a quantity whose Poisson bracket with every one of the ϕ 's vanishes weakly.

Also, we can expand the determinant A in terms of the elements of the first column, and get A as a linear combination of the χ 's. So we have the result that a certain linear combination of the χ 's has zero Poisson brackets with all the ϕ 's. That means that this linear combination of the χ 's is first class. That contradicts our assumption that we have put as many χ 's as possible into the first class. That proves the theorem.

Incidentally, we see that the number of surviving χ 's, which cannot be brought into the first class, must be even, because the determinant Δ is antisymmetrical. Any antisymmetrical determinant with an odd number of rows and columns vanishes. This one doesn't vanish and therefore must have an even number of rows and columns.

Because this determinant, Δ, doesn't vanish, we can bring in the reciprocal $c_{ss'}$ of the matrix whose determinant is Δ. We define the matrix $c_{ss'}$ by

$$c_{ss'}\,[\chi_{s'},\chi_{s'}] = \delta_{ss''} \tag{2-30}$$

We now define new Poisson brackets in accordance with this formalism: any two quantities ξ, η have a new Poisson bracket defined by

$$[\xi,\eta]^* = [\xi,\eta] - [\xi,\chi_s]\,c_{ss'}\,[\chi_{s'},\eta]\,. \tag{2-31}$$

It is easy to check that new Poisson brackets defined in this way satisfy the laws which Poisson brackets usually satisfy: $[\xi,\eta]^*$ is antisymmetrical between ξ and η, is linear in ξ, is linear in η, satisfies the product law $[\xi_1\xi_2,\eta]^* = \xi_1\,[\xi_2\eta]^* + [\xi_1,\eta]^*\,\xi_2$, and obeys the Jacobi identity $[[\xi,\eta]^*,\zeta]^* + [[\eta,\zeta]^*\xi]^* + [[\zeta,\xi]^*,\eta]^* = 0$.

I don't know of any neat way of proving the Jacobi identity for the new Poisson brackets. If one just substitutes according to the definition and works it out in a complicated way, one does find that all the terms cancel out and that the left-hand side equals zero. I think there ought to be some neat way of proving it, but I haven't been able to find it. The straightforward method I have given in the Canadian Journal of Mathematics, 2, 147 (1950). The problem has been dealt with by Bergmann, Physical Review, 98, 531 (1955).

Now let us see what we can do with these new Poisson brackets. First of all, I would like you to notice that the equations of motion are as valid for the new Poisson brackets as for the original ones.

$$\begin{aligned}[g, H_T]^* &= [g, H_T] - [g, \chi_s]\, c_{ss'}\, [\chi_{s'}, H_T] \\ &\approx [g, H_T]\end{aligned}$$

because the terms $[\chi_{s'}, H_T]$ all vanish weakly on account of H_T being first-class. Thus we can write

$$\dot{g} \approx [g, H_T]^* .$$

Now if we take any function ξ whatever of the q 's and p 's, and form its new Poisson bracket with one of the χ 's, say $\chi_{s''}$, we have

$$\begin{aligned}[\xi, \chi_{s''}]^* &= [\xi, \chi_{s''}] - [\xi, \chi_s]\, c_{ss'}\, [\chi_{s'}, \chi_{s''}] \\ &= [\xi, \chi_{s''}] - [\xi, \chi_s]\, \delta_{ss''} \quad \text{by } (2-30) \\ &= 0\end{aligned}$$

Thus we can put the χ 's equal to 0 before working out new Poisson brackets. This means that the equation

$$\chi_s = 0 \tag{2-32}$$

may be considered as a strong equation.

[42]

We modify our classical theory in this way, bringing in these new Poisson brackets, and this prepares the ground for passing to the quantum theory. We pass over to the quantum theory by taking the commutation relations to correspond to the new Poisson bracket relations and taking the strong equations (2-32) to be cquations between operators in the quantum theory. The remaining weak equations, which are all first class, become again supplementary conditions on the wave functions. The situation is then reduced to the previous case where there were only first-class ϕ 's. We have again, therefore, a method of quantizing our general classical Hamiltonian theory. Of course, we again need a bit of luck in order to arrange that the coefficients are all on the left in the consistency conditions.

That gives the general method of quantization. You notice that when we have passed over to the quantum theory, the distinction between primary constraints and secondary constraints ceases to be of any importance. The distinction between primary and secondary constraints is not a very fundamental one. It depends very much on the original Lagrangian which we start off with. Once we have gone over to the Hamiltonian formalism, we can really forget about the distinction between primary and secondary constraints. The distinction between first-class and second-class constraints is very important. We must put as many as possible into the first class and bring in new Poisson brackets which cnable us to treat the surviving second-class constraints as strong.

24.5.4 Dirac's Lecture 3: Quantization on Curved Surfaces

We started off with a classical action principle. We took our action integral to be Lorentz-invariant. This action gives us a Lagrangian. We then passed from the Lagrangian to the Hamiltonian, and then to the quantum theory by following through certain rules. The result is that, starting with a classical field theory, described by an action principle, we end up with a quantum field theory. Now you might think that that finishes our work, but there is one important problem still to be considered: whether our quantum field theory obtained in this way is a relativistic theory. For the purposes of discussion, we may confine ourselves to special relativity. We have then to consider whether our quantum theory is in agreement with special relativity.

We started from an action principle and we required that our action should be Lorentz-invariant. That is sufficient to ensure that our classical theory shall be relativistic. The equations of motion that follow from a Lorentz invariant action principle must be relativistic equations. It is true that when we put these equations of motion into the Hamiltonian form, we are disturbing
the four-dimensional symmetry. We are expressing our equations in the form

$$\dot{g} \approx [g, H_T]\,. \tag{1-21}$$

The dot here means dg/dt and refers to one absolute time, so that the classical equations of motion in the Hamiltonian form are not manifestly relativistic, but we know that they must be relativistic in content because they follow from relativistic assumptions.

However, when we pass over to the quantum theory we are making new assumptions. The expression for H_T which we have in the classical theory does not uniquely determine the quantum Hamiltonian. We have to decide questions about the order in which to put non-commuting factors in the quantum theory. We have something at our disposal in choosing this order, and so we are making new assumptions. These new assumptions may disturb the relativistic invariance of the theory, so that the quantum field theory obtained by this method is not necessarily in agreement with relativity. We now have to face the problem of seeing how we can ensure that our quantum theory shall be a relativistic theory.

For that purpose we have to go back to first principles. It is no longer sufficient to consider just one time variable referring to one particular observer; we have to consider different observers moving relatively to one another. We must set up a quantum theory which applies equally to any of these observers, that is, to any time axis. To get a theory involving all the different time axes, we should first get the corresponding classical theory and then pass from this classical theory to the quantum theory by the standard rules.

I would like to go back to the beginning of our

Hamiltonian development and consider a special case. We started our development by taking a Lagrangian L, which is a function of dynamical coordinates and velocities $q, \dot{q}$, introducing the momenta, then introducing the Hamiltonian. Let us take the special case when L is homogeneous of the first degree in the q 's. Then Euler's Theorem tells us that

$$\dot{q}_n \frac{\partial L}{\partial \dot{q}_n} = L \tag{3-1}$$

That just tells us that $p_n \dot{q}_n - L = 0$. Thus we get in this special case a Hamiltonian that is zero.

We necessarily get primary constraints in this case. There must certainly be one primary constraint, because the p 's are homogeneous functions of degree zero in the velocities. The p 's are thus functions only of the ratios of the velocities. The number of p 's is equal to N, the number of degrees of freedom, and the number of ratios of the velocities is $N - 1$. N functions

of $N-1$ ratios of the velocities cannot be independent. There must be at least one function of the p 's and q 's which is equal to zero; there must be at least one primary constraint. There may very well be more than one. One can also see that, if we are to have any motion at all with a zero Hamiltonian, we must have at least one primary first-class constraint.

We have the expression (1-33) for the total Hamiltonian

$$H_T = H' + v_a\phi_a.$$

H' must be a first-class Hamiltonian, and as 0 is certainly a first-class quantity we may take $H' = 0$. Our total

Ilamiltonian is now built up entirely from the primary first-class constraints with arbitrary coefficients:

$$H_T = v_a\phi_a \tag{3-2}$$

showing that there must be at least one primary firstclass constraint if we are to have any motion at all.

Our equations of motion now read like this:

$$\dot{g} \approx v_a\,[g, \phi_a]$$

We can see that the $\dot{g}$'s may all be multiplied by a factor because, since the coefficients v are arbitrary, we may multiply them all by a factor. If we multiply all the dg/dt 's by a factor, it means that we have a different time scale. So we have now Hamiltonian equations of motion in which the time scale is arbitrary. We could introduce another time variable τ instead of t and use τ to give us equations of motion

$$\frac{dg}{d\tau} \approx v'_a\,[g, \phi_a] \tag{3-3}$$

So we have now a Hamiltonian scheme of equations of motion in which there is no absolute time variable. Any variable increasing monotonically with t could be used as time and the equations of motion would be of the same form. Thus the characteristic of a Hamiltonian theory where the Hamiltonian H' is zero and where every Hamiltonian is weakly equal to zero, is that there is no absolute time.

We may look at the question also from the point of view of the action principle. If I is the action integral, then

$$I = \int L(q, \dot{q})dt = \int L\left(q, \frac{dq}{d\tau}\right)d\tau \tag{3-4}$$

bed use L is homogeneous of the first degree in ti. dq/l^t. So we can express the action integral with respe. to [in] the same form as with respect to t. That show that the equations of motion which follow from the action pris [ciple] must be invariant under the passage from t to τ. The equations of motion do not refer to any absolute tim.

ve have thus a special form of Hamiltonian theory but [in] fact this form is not really so special because, star ing with any Hamiltonian, it is always permissible to ake the time variable as an extra coordinate and brif the theory into a form in which the Hamiltonian is weady equal to zero. The general rule for doing this is the following: we take t and put it equal to another dyn [mical] coordinate q_0. We set up a new Lagrangian

$$L^* = \frac{dq_0}{d\tau} L\left(q, \frac{dq/d\tau}{dq_0/d\tau}\right)$$
$$= L^*\left(q_k, \frac{dq_k}{d\tau}\right), \quad k = 0, 1, 2, ..., N(\tag{3-5}$$

L^* avolves one more degree of freedom than the original L.1* is not equal to L but

$$\int L^* d\tau = \int L dt$$

Thi the action is the same whether it refers to L^* and τ of to L and t. So for any dynamical system we can trea $^{\text{the time as an extra coordinate}}$ q_0 and then pass to a $\mathrm{n}^{\mathbb{N}}$ Lagrangian L^*, involving one extra degree of free $^{\text{om}}$ and homogeneous of the first degree in the veloties. L^* gives us a Hamiltonian which is weakly equ to zero.
T^{is} special case of the Hamiltonian formalism where

Ur llamiltonian is weakly equal to zero is what we need In a relativistic theory, because in a relativistic theory wr don't want to have one particular time playing a elucial role; we want to have the possibility of various turnes τ which are all on the same footing. Let us see in detail how we can apply this idea.

We want to consider states at specified times with (w) pect to different observers. Now if we set up a spacetome picture as in Fig. 1, the state at a certain time refers (1) the physical conditions on a three-dimensional flat arace-like surface S_1 which is orthogonal to the time axis. The state at different times will refer to physical conditions on different surfaces $S_2, S_3, ...$ Now we want to bring in other time axes referring to different observers and the state, with respect to the other time .xes, will involve physical conditions on other flat upace-like surfaces like S_1'. We want to have a Hamiltonban theory which will enable us to pass from the state, S_1 say, to the state S_1'. Starting off with given initial conditions on the surface S_1 and applying the equations of motion, we must be able to pass over to the physical conditions on the surface S_1^f. There must thus be four freedoms in the motion of a state, one freedom corresponding to the movement of the surface parallel to itself, then three more freedoms corresponding to a general change of direction of this flat surface. That means that there will be four arbitrary functions occurring in the solution of the equations of motion which we are trying to get. So we need a Hamiltonian theory with (at least) four primary first-class constraints.

There may be other primary first-class constraints if there are other kinds of freedom in the motion, for example, if we have the possibility of the gauge

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transformations of electrodynamics. To simplify the discussion, I will ignore this possibility of other firstclass primary constraints, and consider only the ones which arise from the requirements of relativity.

We could proceed to set up our theory referring to these flat space-like surfaces which can move with the four freedoms, but I would like first to consider a more

Figure 2

general theory in which we consider a state to be defined on an arbitrary curved space-like surface, such as S of Fig. 2. This represents a three-dimensional surface in space-time which has the property of being everywhere space-like, that is to say, the normal to the surface must lie within the light-cone. We may set up a Hamiltonian theory which tells us how the physical conditions

vary when we go from one of the curved space-like surfaces to a neighboring one.

Now, bringing in the curved surfaces means bringing in something which is not necessary from the point of view of special relativity. If we wanted to bring in general relativity and

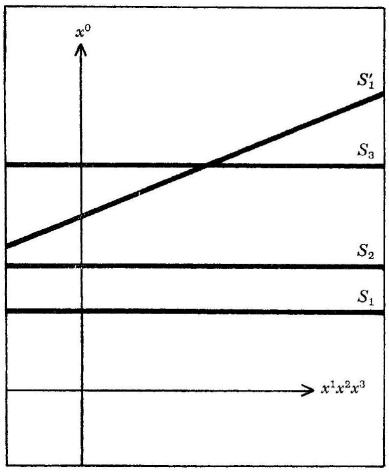
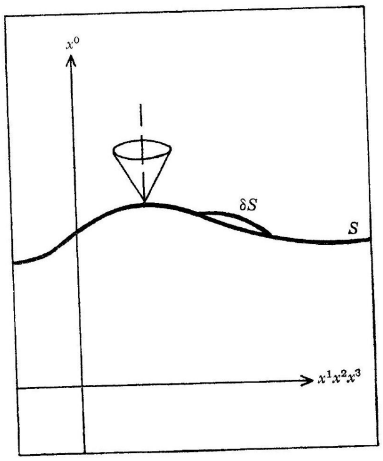


Figure 1



gravitational fields, then it would be essential to work with these curved surfaces, but for special relativity, the curved surfaces are not essential. However, I like to bring them in at this stage, even for the discussion of a theory in special relativity, because I find it easier to explain the basic ideas with reference to these curved surfaces than with reference to the flat surfaces. The reason is that with these curved surfaces we can make local deformations of the surface like δS in Fig. 2, and discuss the equations of motion with respect to these local deformations of the surface.

One way of proceeding now would be to refer our action integral to a set of curved surfaces, like S, take the amount of action between two neighboring curved surfaces, divide it by some parameter $\delta\tau$ expressing the distance between these two surfaces, take this amount of action as our Lagrangian, then apply our standard method of passing from the Lagrangian to the Hamiltonian. Our Lagrangian would necessarily be homogeneous of the first degree in the velocities with respect to the time parameter τ which specifies the passage from one of these space-like surfaces to a neighboring one, and it would lead to a Hamiltonian theory for which the Hamiltonian is weakly equal to zero.

However, I don't want to go through all the work of following through in detail what we get from an action principle. I want to short-circuit that work and discuss the form of the final Hamiltonian theory which results.

We can get quite a lot of information about the form of this Hamiltonian theory just from our knowledge that there must be freedom for the space-like surface to move arbitrarily so

long as it remains always space-like. This freedom of motion of the space-like surface must correspond to first-class primary constraints in the Hamiltonian, there being one primary first-class constraint for each type of elementary motion of the surface which can be set up. I shall develop the theory from that point of view.

First of all we have to introduce suitable dynamical variables. Let us describe a point on the space-like surface S by three curvilinear coordinates $(x^1, x^2, x^3) = (x^r)$. In order to fix the position of this space-like surface in space-time, we introduce another set of coordinates $y_A (\Lambda = 0, 1, 2, 3)$, which we may take to be rectilinear, orthogonal coordinates in special relativity. (I use a capital suffix for referring to the y coordinate system and a small suffix such as r for referring to the x coordinate system.) The four functions y_A, of x^r, will specify the surface S in space time and will also specify its parameterization, i.e. the system of coordinates x^1, x^2, x^3.

We can use these y_A as dynamical coordinates, q 's. If we form

$$y_{\Lambda,r} = \frac{\partial y_\Lambda}{\partial x^r}, \quad (r = 1, 2, 3) \tag{3-6}$$

this is a function of the q 's, the dynamical coordinates.

$$\dot{y}_\Lambda = \frac{\partial y_\Lambda}{\partial \tau} \tag{3-7}$$

τ being the parameter changing from one surface to the neighboring surface, will be a velocity, a $\dot{q}$. Thus y_A are the dynamical coordinates needed for describing the surface and $\dot{y}_A$ are the velocities.

We shall need to introduce momentum variables w_A conjugate to these dynamical coordinates. The momentum variables will be connected with the coordinates by the Poisson bracket relations

$$[y_{Ax}, w_{\Gamma x'}] = g_{A\Gamma} \delta^3 (x - x') . \tag{3-8}$$

We shall need other variables for describing any physical fields which occur in the problem. If we are dealing with a scalar field V, then $V(x)$ for all values of x^1, x^2, x^3 will provide us with further dynamical coordinates, q 's. $V_{,r}$ will be functions of the q 's. $\partial V/\partial \tau$ will be a velocity. The derivative of V in any direction is expressible of terms of $\hat{\varepsilon} V/\hat{c}\tau$ and $V_{,r}$ and so is expressible in terms of the dynamical coordinates and velocities. The Lagrangian will involve these V 's differentiated in general directions and is thus a function of the dynamical coordinates and velocities. For each V, we shall need a conjugate momentum U, satisfying the Poisson bracket conditions

$$[V(x), U(x')] = \delta^3 (x - x') . \tag{3-9}$$

That is how one would treat a scalar field. There is a similar method for vector, tensor, or spinor fields, just bringing in the necessary additional suffixes. I need not go into that.

Now let us see what the Hamiltonian will be like. The Hamiltonian has to be a linear function of primary first-class constraints of the type (3-2). First of all I shall put down what the primary first-class constraints are like. There must be primary first-class constraints which allow for arbitrary deformations of the surface. They must involve the variables w which are conjugate to the y 's, in order to make the y 's vary, and they will involve other field quantities. We can express them in the form

$$w_A + K_A \approx 0, \tag{3-10}$$

where K_Λ is some function of the Hamiltonian variables, the q 's and p 's, not involving the w 's.

Now we can assert that the Hamiltonian is just an arbitrary linear function of all the quantities (3-10):

$$H_T = \int c^\Lambda \left(w_\Lambda + K_\Lambda\right) d^3x \tag{3-11}$$

This is integrated over the three x 's which specify a point on the surface. The c 's are arbitrary functions of the three x 's and the time.

The general equation of motion is of course $\dot{g} \approx [g, H_T]$. We can get a meaning for the coefficient c^A by taking this cquation of motion and applying it for g equal to one of the y variables. For $g = y_A$ at some particular point x^1, x^2, x^3 we get

$$\begin{aligned} \dot{y}_\Lambda &= \left[y_\Lambda, \int c'^T \left(w'_\Gamma + K'_\Gamma\right) d^3x'\right] \\ &= \int c'^T \left[y_\Lambda, w'_\Gamma + K'_\Gamma\right] d^3x \end{aligned} \tag{3-12}$$

Here the ' attached to a field quantity c^Γ, w_Γ or K_Γ denotes the value of that quantity at the point $X^{1'}, X^{2'}, X^{3'}$. y_A has zero Poisson brackets with K'_T because K'_T is independent of the w 's, so we just have to take into

account the Poisson bracket of y_A with $w'_\Gamma = w_\Gamma\left(x'\right)$ This gives us the delta function and so

$$\dot{y}_A = c_A. \tag{3-13}$$

Thus the coefficients c_A turn out to be the velocity variables which tell us how our surface varies with the parameter τ. We can get an arbitrary variation of the surface with τ by choosing these c_A in an arbitrary way.

This tells us what the Hamiltonian is like for a field theory expressed with respect to states on curvilinear surfaces.

We can make a deeper analysis of this Hamiltonian by resolving the vectors which occur in it into components which are normal and tangential to the surface. If we have any vector whatever, ξ_A, we can obtain from ξ_A a normal component

$$\xi_\perp = \xi_A l^\Lambda$$

where l^4 is the unit normal vector, and tangential components (referred to the x coordinate system)

$$\xi_r = \xi_A y^A_{,r}$$

The l are determined by the $y^A_{,r}$ and are thus functions of the dynamical coordinates. Any vector can be resolved in this way into a part normal to the surface and a part tangential to the surface. We have the scalar product law

$$\xi_\Lambda \eta^\Lambda = \xi_\perp \eta_\perp + \gamma^{rs} \xi_r \eta_s \tag{3-14}$$

where $\gamma_{rs} dx^r dx^s$ is the metric in the surface referred to the x-coordinate system. γ^{rs} is the reciprocal matrix of the γ_{rs}.$(r, s = 1, 2, 3)$.

We can use this scalar product law (3-14) to express

our total Hamiltonian in terms of the tangential and normal components of w and K :

$$H_T = \int \dot{y}^\Lambda \left(w_A + K_\Lambda\right) d^3x$$
$$= \int \left(\dot{y}_\perp \left(w_\perp + K_\perp\right) + \gamma^{rs}\dot{y}_r \left(w_s + K_s\right)\right) d^3x \tag{3-15}$$

Here $\dot{y} = \dot{y}^A l_A$ and $\dot{y}_r = \dot{y}^A y_{A,r}$.
We shall need the Poisson bracket relationships between the normal and tangential terms in (3-15). I will first write down the Poisson bracket relations for the different components of w. We have of course

$$[w_A, w'_\Gamma] = 0 \tag{3-16}$$

referred to the external coordinates y; but when we resolve our w 's into normal and tangential components, they will no longer have zero Poisson brackets with each other. The Poisson brackets can easily be worked out by straightforward arguments. I don't want to go through the details of that work. I will just mention that the details can be found in a paper of mine (Canadian Fournal of Mathematics, 3, 1 (1951)). The results are

$$[w_r, w'_s] = w_s \delta_r \left(x - x'\right) + w'_r \delta_s \left(x - x'\right) \tag{3-17}$$
$$[w_\perp, w'_r] = w'_\perp \delta_r \left(x - x'\right) \tag{3-18}$$
$$[w_\perp, w'_\perp] = -2w^r \delta_r \left(x - x'\right) - w^r_r \delta \left(x - x'\right) \tag{3-19}$$

Now we know that

$$[w_\mu + K_\mu, w'_\nu + K'_\nu] \approx 0 \quad \text{for } \mu, \nu = r, s \text{ or } \perp . \tag{3-20}$$

We can infer that

$$[w_r + K_r, w'_s + K'_s]$$
$$= \left(w_s + K_s\right) \delta_{,r} \left(x - x'\right) + \left(w'_r + K'_r\right) \delta_{,s} \left(x - x'\right)$$
$$[w_\perp + K_\perp, w'_r + K'_r] \qquad ((3-21;)$$
$$= \left(w'_\perp + K'_\perp\right) \delta_{,r} \left(x - x'\right), \tag{3-22}$$
$$[w_\perp + K_\perp, w'_\perp + K'_\perp]$$
$$= -2\left(w^r + K^r\right) \delta_{,r} \left(x - x'\right) - \left(w^r + K^r\right)_{,r} \delta \left(x - x'\right). \tag{3-23}$$

These results could be worked out directly from the definitions of the normal and tangential components of the w 's, but they can be inferred more simply by the following argument. Since $w_r + K_r, w_\perp + K_\perp$ are all first class, their Poisson brackets are zero weakly. Thus $[w_r + K_r, w'_s + K'_s], [W_\perp + K_\perp, w'_r + K'_r]$ and $[w. \ + K_\perp, \mathfrak{w}'_\perp + K'_\perp]$ must all be weakly equal to zero. We can now infer what they are equal to strongly. We have to put on the right-hand side in each of (3-21,) (3-22,) and (3-23) a quantity which is weakly equal to zero and which is therefore built up from $w_r + K_r$ and $w_\perp + K_\perp$ with certain coefficients. Further, we can see what these coefficients are by working out what terms containing w there are on the right-hand sides. Terms containing w's can arise only from taking the Poisson bracket of a w with a w, according to (3-17), (3-18), and (3-19). Taking a Poisson bracket $[\ w, K'\ ]$ will not lead to anything involving w, because it means taking the Poisson bracket of a w momentum with some functions of dynamical coordinates and momenta other than w 's, and that won't involve the w momentum variables. Similarly the Poisson bracket of a K with a K won't involve any

w variables. Thus the only w variables which occur on the right side of (3-21) will be the ones which occur on the right side of (3-17). We have to put certain further terms in the ught side of (3-21) in order that the total expression whall be weakly equal to zero. It is then quite clear what we should put here, namely, $(w_s + K_s)\,\delta_r\,(x - x') + (ww'_r + K'_r)\,\delta_{,s}\,(x - x')$. We do the same with the right :ides of (3-22), (3-23).

The next thing to notice is that the terms $w_s + K_s$ in the Hamiltonian (3-15) correspond to a motion in which we change the system of coordinates in the curved wurface but do not have the surface moving. It correponds to each point in the surface moving tangentially to the surface.

Let us put $\dot{y}_\perp = 0$, which means that we are taking no motion of the surface perpendicular to itself but are merely making a change of the coordinates of the surface, and then we have equations of motion of the type

$$\dot{g} = \int \gamma^{rs}\dot{y}_r\,[g, w_s + K_s]\,d^3x \tag{3-24}$$

This must be the equation of motion which tells us how g varies when we change the system of coordinates in the surface without moving the surface itself. Now this change in g must be a trivial one, which can be inferred merely from the geometrical nature of the dynamical variable g. If g is a scalar, then we know how that changes when we change the system of coordinates x^1, x^2, x^3. If it is a component of a vector or a tensor there will be a rather more complicated change for g, but still we can work it out; similarly if g is a spinor. In every case, this change of g is a trivial one. That means that K_s can be determined from geometrical arguments only.

I will give one or two examples of that. For a scal field V with a conjugate momentum U, there is a ter,

$$V_{,r}U \tag{5}$$

in K_r. For a vector field, say a three-vector A_s, wit conjugate B^s, there is a term

$$A_{s,r}B^s - (A_rB^s)_{,s} \tag{3-26}$$

in K_r; and so on for tensors, with something rather mort complicated for spinors. The first term in (3-26) is th: change in A_s coming from the translation associated with the change in the system of coordinates, and the second is the change in the A_s arising from the rotation associated with the change in the system of coordinates. There is no such rotation term coming in in the case (3-25) of the scalar.

We can obtain the total K_r by adding the contribution needed for all the different kinds of fields which are present in the problem. The result is that we can work out this tangential component of K just from geometrical arguments. One can see in this way that the tangential component of K is something which is not of real physical importance, it is just concerned with the mathematical technique. The quantity which is of real physical importance is the normal component of K in (3-15). This normal component of K added on to the normal component of w gives us the first-class constraint which is associated with a motion of the surface normal to itself. That is something which is of dynamical importance.

The problem of getting a Hamiltonian field theory on these curved surfaces involves finding the expressions K to satisfy the required Poisson bracket relations

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(1-21), (3-22), and (3-23). The tangential part of K can lic worked out from geometrical arguments as I discussed, and when we have worked it out we should find of course that it satisfies the first Poisson bracket relation (3-21). The second Poisson bracket relation (3-22)

involves $K_\perp$ lumearly and this Poisson bracket relation would be mutisfied by any quantity $K_\perp$ which satisfies the condition if being a scalar density. This Poisson bracket relation wally tells us that if the quantity $K_\perp$ varies suitably under . change of coordinate system X^1, X^2, X^3, this Poisson bracket relation will be fulfilled. The difficult relation to tulfill is the third one, which is quadratic in K_1. So the problem of setting up a Hamiltonian field theory on curved space-like surfaces is reduced to the problem of finding a normal component of K which is a scalar density and which satisfies the Poisson bracket relationship (3-23).

One way of finding such a normal component of K is to work from a Lorentzinvariant action principle. We might obtain all the components of K by working from the action principle. If we did that, the tangential part of K which we get would not necessarily be the same as that built up from terms like (3-25) and (3-26), because it might differ by a contact transformation. But one could eliminate such a contact transformation by rewriting the action principle, adding to it a perfect differential term. This doesn't affect the equations of motion. By such a change of the action principle, one can arrange that the tangential part of K given by the action principle agrees precisely with the value which is obtained by the simple application of geometrical arguments. We are then able to find the normal component of K by working with our general method of passing from the action principle to

the Hamiltonian. If the action principle is relativistic, then the normal component of K obtained in this way would have to satisfy the condition (3-23).

We can now discuss the passage to the quantum theory. Quantization involves making the quantities w and the variables which enter in K into operators. We have to be careful now how we define the tangential and the normal components of w, and I choose this way to define them:

$$w_r = y_{\Lambda,r} w^\Lambda \tag{3-27}$$

putting the momentum variable w on the right. (In the quantum theory, you see, the result is different, depending on whether we put the w on the right or the left.) Similarly,

$$w_\perp = l_\Lambda w^\Lambda \tag{3-28}$$

Then these quantities are well defined.
Now in the quantum theory we have the weak equations $w_r + K_r \approx 0$ and $w_\perp + K_\perp \approx 0$, which provide us with supplementary conditions on the wave function:

$$(w_r + K_r)\,\psi = 0 \tag{3-29}$$

$$(w_\perp + K_\perp)\,\psi = 0 \tag{3-30}$$

corresponding to (2-22). We require that these supplementary conditions be consistent. According to (2-25), we must arrange that in the commutation relations (3-21), (3-22), and (3-23) the coefficients on the righthand sides stand before (on the left of) the constraints.

In the case of (3-21), the tangential components, the conditions fit if we choose the order of the factors in K_r so that the momentum variables are always on the right. We have now in (3-21) a number of quantities,

linear in the momentum variables with the momentum variables on the right, and the commutator of any two such quantities will again be linear in the momentum variables with the momentum variables on the right. Thus we shall always have the momentum variables on the right and we shall always have our factors occurring in the order in which we want them to.

Now we have the problem of bringing in $K_\perp$, which cannot be disposed of so simply. $K_\perp$ will usually involve the product of non-commuting factors and we have to arrange the order of

those factors so that (3-22) and (3-23) shall be satisfied with the coefficients occurring on the left in every term on the right-hand side. The equation (3-22) is again a fairly simple one to dispose of. If we simply take $K_\perp$ to be a scalar density, that is all that is needed, because we have $w_\perp + K_\perp$ occurring on the right-hand side without any coefficients which don't commute with it; the only coefficient is the delta function, which is a number.

But the relationship (3-23) is the troublesome one. For the purposes of the quantum theory, I ought to write out the right-hand side here rather more explicitly:

$$[w_\perp + K_\perp, w'_\perp + K'_\perp] = -2\gamma^{rs}\,(w_s + K_s)\,\delta_{,r}\,(x - x') \\ -\left(\gamma^{rs}\,(w_s + K_s)\right)_{,r}\,\delta\,(x - x') \tag{3-31}$$

I've written this out with the coefficients γ^{rs} occurring on the left, and that is how we need to have these coefficients in the quantum theory.

The problem of setting up a quantum field theory on general curved surfaces involves finding $K_\perp$ so that this Poisson bracket relationship (3-31) holds with the coefficients $\gamma^{\tau s}$ occurring on the left. If we do satisfy (3-31),

then the supplementary conditions (3-30) are consistent with each other, and we already have (3-29) consistent with each other and (3-30) consistent with (3-29).

There we have formulated the conditions for our quantum theory to be relativistic. We need a bit of luck to be able to satisfy the conditions. We cannot always satisfy them. There is one general rule which is of importance, which tells us that when we've got a $K_\perp$ satisfying these conditions and certain other conditions, we can easily construct other $K_\perp$'s to satisfy the conditions. Let us suppose that we have a solution in which $K_\perp$ involves only undifferentiated momentum variables together with dynamical coordinates which may be differentiated. There are a number of simple fields for which $K_\perp$ does satisfy the Poisson bracket relations (3-22) and (3-23) and does have this simple character. Then we may add to $K_\perp$ any function of the undifferentiated q 's. That is to say, we take a new K_1,

$$K^*_\perp = K_\perp + \phi(q).$$

Then we see that adding on this ϕ to $K_\perp$ can affect the right-hand side of (3-31) only by bringing in a multiple of the delta function. We cannot get any differentiations of the delta function coming in, because the extra terms come from Poisson brackets of $\phi(q)$ with undifferentiated momentum variables. So that the only effect on the right-hand side of adding the term ϕ to $K_\perp$ can be adding on a multiple of the delta function. But the right-hand side has to be antisymmetrical between x and x', because the left-hand side is obviously antisymmetrical between x and x'. That prevents us from just adding a multiple of the delta function to the right-hand side of (3-31), so that it is not altered at all. Thus if the

original $K_\perp$ satisfies the Poisson bracket relation (3-31), then the new one will also satisfy it.

There is a further factor which has to be taken into account to complete the proof. ϕ may also involve $\Gamma = \sqrt{-\det g_{rs}}$. One finds that $[w_1, \Gamma']$ involves $\delta\,(x - x')$ undifferentiated (one just has to work this out) and thus we can bring Γ into ϕ without disturbing the argument. In fact, we have to bring in Γ in order to preserve the validity of (3-22), which requires that $K^*_\perp$ and $K_\perp$ shall be scalar densities. We must thus bring in a suitable power of Γ to make ϕ a scalar density.

This is the method which is usually used in practice for bringing in interaction between fields without disturbing the relativistic character of the theory. For various simple fields the conditions turn out to be satisfied. We have the necessary bit of luck, and we can bring in interaction between fields of the simple character described and the conditions for the quantum theory to be relativistic are preserved.

There are some examples for which we don't have the necessary luck and we just cannot arrange the factors in $K_\perp$ to get (3-31) holding with the coefficients on the left, and then we do not know how to quantize the theory with states on curved surfaces. But actually, we are trying to do rather more than is necessary when we try to set up our quantum theory with states on curved surfaces. For the purposes of getting a theory in agreement with special relativity, it would be quite sufficient to have our states defined only on flat surfaces. That will involve some conditions on $K_\perp$ which are less stringent than those which I have formulated here. And it may be that we can satisfy these less stringent conditions without being able to satisfy those which I have formulated here.

An example for that is provided by the Born-Infeld electrodynamics, which is a modification of the Maxwell electrodynamics based on a different action integral, an action integral which is in agreement with the Maxwell one for weak fields, but differs from it for strong fields. This Born-Infeld electrodynamics leads to a classical $K_\perp$ which involves square roots. It is of such a nature that it doesn't seem possible to fulfill the conditions which are necessary for building up a relativistic quantum theory on curved surfaces. However, it does seem to be possible to build up a relativistic quantum theory on flat surfaces, for which the conditions are less stringent.

24.5.5 Dirac's Lecture 4: Quantization on Flat Surfaces

We have been working with states on general space-like curved surfaces in space-time. I will just summarize the results that we obtained concerning the conditions for a quantum field theory, formulated in terms of these states, to be relativistic. We introduce variables to describe the surface, consisting of the four coordinates y^Λ of each point $x^r = (x^1, x^2, x^3)$ on the surface. The x 's form a curvilinear system of coordinates on the surface. Then the y 's are treated as dynamical coordinates and there are momenta conjugate to them, $w_A(x)$, again functions of the x 's. And then we get a number of primary first-class constraints appearing in the Hamiltonian formalism, of the nature

$$w_\Lambda + K_\Lambda \approx 0 \tag{3-10}$$

The K 's are independent of the w 's, but may be functions of any of the other Hamiltonian variables. The K 's will involve the physical fields which are present. We analyze these constraints by resolving them into components tangential to the surface and normal to the surface. The tangential components are

$$w_r + K_r \approx 0 \tag{4-1}$$

and the normal component is

$$w_\perp + K_\perp \approx 0 \tag{4-2}$$

With this analysis, we find that the K_r can be worked out just from geometrical considerations. The K_r should be looked upon as something rather trivial, associated with transformations in which the coordinates of the surface are varied, but the surface itself doesn't move. The first-class constraints (4-2) are associated with the motion of the surface normal to itself and are the important ones physically.

Certain Poisson bracket relations (3-21), (3-22), and (3-23) have to be fulfilled for consistency. Some of the Poisson bracket relations involve merely the K_r, and they are automatically satisfied when the K_r are chosen in accordance with the geometrical requirements. Some of the consistency conditions are linear in $K_\perp$ and they are automatically satisfied provided we choose $K_\perp$ to be a scalar density. Then finally we have the consistency conditions which are

quadratic in the $K_\perp$ and those are the important ones, the ones which cannot be satisfied by trivial arguments.

These important consistency conditions can be satisfied in the classical theory if we work from a Lorentzinvariant action principle and calculate the $K_\perp$ by following the standard rules of passing from the action principle to the Hamiltonian. The problem of getting a relativistic quantum theory then reduces to the problem of suitably choosing the non-commuting factors which occur in the quantum $K_\perp$ in such a way that the quantum consistency conditions are fulfilled, which means that the commutator of two of the quantities (4-2) at two points in space x^1, x^2, x^3 has to be a linear combination of the

constraints with coefficients occurring on the left. These quantum consistency conditions will usually be quite difficult to satisfy. It turns out that one can satisfy them with certain simple examples, but with more complicated examples it doesn't seem to be possible to satisfy them. That leads to the conclusion that one cannot set up a quantum theory for these more general fields with the states defined on general curved surfaces.

I might mention that the quantities K have a simple physical meaning. K_r can be interpreted as the momentum density, $K_\perp$ as the energy density; so the momentum density, expressed in terms of Hamiltonian variables, is something which is always easy to work out just from the geometrical nature of the problem and the energy density is the important quantity which one has to choose correctly (satisfying certain commutation relations) in order to satisfy the requirements of relativity.

If we cannot set up a quantum theory with states on general curved surfaces, it might still be possible to set it up with states defined only on flat surfaces.

We can get the corresponding classical theory simply by imposing conditions which make our previous curved surface into a flat surface. The conditions will be the following: The surface is specified by $y_\Lambda(x)$; in order to make the surface flat, we require that these functions shall be in the form

$$y_A(x) = a_A + b_{\Lambda r} x^r \tag{4-3}$$

where the a 's and b 's are independent of the x 's. This will result in the surface being flat, and in the system of coordinates x^r being rectilinear. At present we are not imposing the conditions that the x^r coordinate system shall be orthogonal: I shall bring that in a little later. [69]

We are thus working with general, oblique, rectilinear axes x^r.

We now have our surface fixed by quantities a_A, b_{Ar} and these quantities will appear as the dynamical variables needed to fix the surface. We have far fewer of them than previously. In fact, we have only $4 + 12 = 16$ variables here. We have these 16 dynamical coordinates to fix the surface instead of the previous $y_A(x)$, which meant $4 \cdot \infty^3$ dynamical coordinates.

When we restrict the surface in this way, we may look upon the restriction as bringing a number of constraints into our Hamiltonian formalism, constraints which express the $4 \cdot \infty^3 y$ coordinates in terms of 16 coordinates. These constraints will be second-class. Their presence means a reduction in the number of effective degrees of freedom for the surface from $4 \cdot \infty^3$ to 16 , a very big reduction!

In a previous lecture I gave the general technique for dealing with second-class constraints. The reduction in the number of effective degrees of freedom leads to a new definition of Poisson brackets. This general technique is not needed in our present case, where conditions are sufficiently simple for one to be able to use a more direct method. In fact, we can work out directly what effective momentum variables remain in the theory when we have reduced the number of effective degrees of freedom for the surface.

With our dynamical coordinates restricted in this way, we have of course the velocities restricted by the equation

$$\dot{y}_A = \dot{a}_A + b_{\Lambda r} x^r. \tag{4-4}$$

The dot refers to differentiation with respect to some parameter τ. As τ varies, this flat surface varies, moving

parallel to itself and also changing its direction. The surface thus moves with a four-fold freedom, and this motion is expressed by our taking a_A, b_{Ar} to be functions of the parameter τ.

The total Hamiltonian is now

$$\begin{aligned} H_T &= \int \dot{y}^A \left(w_\Lambda + K_\Lambda\right) d^3x \\ &= \dot{a}^A \int \left(w_\Lambda + K_\Lambda\right) d^3x + b_r^A \int x^r \left(w_\Lambda + K_\Lambda\right) d^3x \end{aligned} \tag{4-5}$$

(I have taken the quantities $\dot{a}^A, b^\Lambda$. outside the integral signs, because they are independent of the x variables.) (4-5) involves the w variables only through the combinations $\int w_\Lambda d^3x$ and $\int x^r w_\Lambda d^3x$. We have here 16 combinations of the w 's, which will be the new momentum variables conjugate to the 16 variables a, b which are now needed to describe the surface.

We can again express H_T in terms of the normal and tangential components of these quantities:

$$\begin{aligned} H_T = \dot{a}^\Lambda l_\Lambda \int \left(w_\perp + K_\perp\right) d^3x + \dot{a}^\Lambda b_{\Lambda r} \int \left(w^r + K^r\right) d^3x \\ + b_r^\Lambda l_\Lambda \int x^r \left(w_\perp + K_\perp\right) d^3x + b_{\Lambda r} b_{\mathrm{s}}^\Lambda \int x^r \left(w^s + K^8\right) d^3x \end{aligned} \tag{4-6}$$

Let us now bring in the condition that the x^r coordinate system is orthogonal. That means

$$b_{\Lambda r} b_s^\Lambda = g_{rs} = -\delta_{rs}. \tag{4-7}$$

Differentiating (4-7) with respect to τ, we get

$$b_{\Lambda r} b_s^\Lambda + b_{\Lambda s} b_r^\Lambda = 0$$
$$\left[7^1\right]$$

(I have been raising the Λ suffixes quite freely because the Λ coordinate system is just the coordinate system of special relativity.) This equation tells us that $b_{Ar} b_s^\Lambda$ is antisymmetric between r and s. So the last term in (4-6) is equal to

$$\frac{1}{2} b_{\Lambda r} b_s^A \int \left\{x^r \left(w^s + K^s\right) - x^s \left(w^r + K^r\right)\right\} d^3x$$

Now you see that we don't have so many linear combinations of the w's occurring in the H_T as before. The only linear combinations of the w's which survive are the following ones:

$$P_\perp \equiv \int w_\perp d^3x, \tag{4-9}$$

$$P_r \equiv \int w_r d^3x, \tag{4-10}$$

$$\text{and also} \quad M_{r\perp} \equiv \int x^r w_\perp d^3x, \tag{4-11}$$

$$\text{and} \quad M_{rs} \equiv \int \left(x_r w_s - x_s w_r\right) d^3x. \tag{4-12}$$

(We can raise and lower the suffixes r quite freely now because they refer to rectilinear orthogonal axes.) These are the momentum variables which are conjugate to the variables needed to fix the surface when the surface is restricted to be a flat one referred to rectilinear orthogonal coordinates.

The whole set of momentum variables included in (4-9), (4-10), (4-11), and (4-12) can be written as P_μ and $M_{\mu\nu} = -M_{\nu\mu}$, where the suffixes μ and ν take on 4 values, a value 0 associated with the normal component, and $1, 2, 3$ associated with the three x 's. μ, ν are small

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suffixes referring to the x coordinate system, to distinguish them from the capital suffixes Λ referring to the fixed y coordinate system.

So now our momentum variables are reduced to just 10 in number, and associated with these 10 momentum variables we have 10 primary first-class constraints, which we may write

$$P_\mu + p_\mu \approx 0 \tag{4-13}$$

$$M_{\mu\nu} + m_{\mu\nu} \approx 0 \tag{4-14}$$

$$\text{where } p_\perp \equiv \int K_\perp d^3x$$

$$p_r \equiv \int K_r d^3x \tag{4-15}$$

$$m_{r\perp} \equiv \int x_r K_\perp d^3x \tag{4-16}$$

$$\text{and} \tag{4-17}$$

$$m_{rs} \equiv \int (x_r K_s - x_s K_r)\, d^3x \tag{4-18}$$

We have now 10 primary first-class constraints associated with a motion of the flat surface. In Lecture (3) I said that we would need 4 primary first-class constraints ($3 - 10$) to allow for the general motion of a flat surface. We see now that 4 is not really adequate. The 4 has to be increased to 10 , because 4 elementary motions of the surface normal to itself and changing its direction would not form a group; in order to have these elementary motions forming a group, we have to extend the 4 to 10 , the extra 6 members of the group including the translations and rotations of the surface, which motions affect merely the system of coordinates in the surface without affecting the surface as a whole. In this

way we are brought to a Hamiltonian theory involving 10 primary firstclass constraints

We have now to discuss the consistency conditions, the conditions in terms of Poisson bracket relations which are necessary for all the constraints to be first classLet us first discuss the Poisson bracket relations between the momentum variables $P_\mu, M_{\mu v}$ We are given these momentum variables in terms of the w variables 4 nd we know the Poisson bracket relations (317) , (318) ,and (319) between the w variables,so we can calculate the Poisson bracket relations between the P and M variablesIt is not really necessary to go through all this work to determine the Poisson bracket relations between the P and M variables It is sufficient to realize that these variables just corre spond to the operators of translation and rotation in four dimensional flat spacetime,and thus their Poisson bracket relations must just correspond to the commuta tion relations between the operators of translation and rotationIn either way we get the following Poisson bracket relations

$$[P_u, P_v] = 0 \tag{4-19}$$

which expresses that the various translations commute

$$[P_\mu, M_{\rho\sigma}] = g_{\mu\rho}P_\sigma - g_{\mu\sigma}P_\rho; \tag{4-20}$$
$$\text{and} \quad [M_{\mu\nu}, M_{\rho\sigma}] = -g_{\mu\rho}M_{v\sigma} + g_{v\rho}M_{\mu\sigma} + g_{\mu\sigma}M_{v\rho} - g_{v\sigma}M_{\mu\rho}.$$

Let us now consider the requirements for the equations (413) and (414) to be firstclassThe Poisson bracket of any two of them must be something which vanishes weakly and must therefore be a linear combination of

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themSo we are led to these Poisson bracket relations

$$[P_\mu + p_\mu, P_v + p_v] = 0,(4-22) \tag{4-22}$$
$$[P_\mu + p_\mu, M_{\mu\sigma} + m_{\mu\sigma}] = g_{\mu\rho}\left(P_\sigma + p_\sigma\right) - g_{\mu\sigma}\left(P_\rho + p_\rho\right), \tag{4-23}$$
$$\text{and } [M_{\mu\nu} + m_{\mu\nu}, M_{\rho\sigma} + m_{\rho\sigma}] = -g_{\mu\rho}\left(M_{\nu\sigma} + m_{\nu\sigma}\right) + g_{\nu\rho}\left(M_{\mu\sigma} + m_{\mu\sigma}\right) + g_{\mu\sigma}\left(M_{\nu\rho} + m_{\nu\rho}\right) - g_{\nu\sigma}\left(M_{\mu\rho} + m_{\mu\rho}\right).(4-24) \tag{4-24}$$

The argument for getting these relations is that,on the righthand sides we had to put something which is weakly equal to zero in each case,and we know the terms on the righthand sides which involve the momentum variables P, M because these terms come only from the Poisson brackets of momenta with momenta and so are given by (419) , (420) ,and (421) (I have already used the same argument in the curvilinear case for (321) , (322) ,and (323) ,so there is no need to go into detail hereFor example,see how (423) comes aboutThe terms involving P are just the same as in (420) They come from the Poisson bracket of P and M The remain ing terms are filled in in order to make the total expres sion weakly equal to zero) (422) , (423) ,and (424) are the requirements for consistency

We can make a further simplification,which we could not do in the case of curvilinear coordinates,in this way Let us suppose that our basic field quantities are chosen to refer only to the x coordinate systemThey are field quantities at specific points x in the surface,and we can choose them so as to be quite independent of the y coordinate systemThen the quantities $K_\perp, K_r$ will be quite independent of the y coordinate system,and that means that they will have zero Poisson brackets with the

variables P, M. We then have a zero Poisson bracket between each of the variables p, m and each of the P, M.

This condition follows with the natural choice of dynamical variables to describe the physical fields which are present. We cannot do the corresponding simplification when we are working with the curved surfaces, because the g_{rs} variables that fix the metric will enter into the quantities $K_\perp, K_r$. The result is that we cannot set them up in a form which does not refer at all to the y coordinate system, because the y coordinates enter into the g_{rs} variables. However, with the flat surfaces, we can make this simplification, and that results in equations (4-22), (4-23), and (4-24) simplifying to

$$[p_\mu, p_\nu] = 0; \tag{4-25}$$
$$[p_\mu, m_{\rho\sigma}] = g_{\mu\rho}p_\sigma - g_{\mu\sigma}p_\rho; \tag{4-26}$$

and

$$[m_{\mu\nu}, m_{\rho\sigma}] = -g_{\mu\rho}m_{\nu\sigma} + g_{\nu\rho}m_{\mu\sigma} + g_{\mu\sigma}m_{\nu\rho} - g_{\nu\sigma}m_{\mu\rho}. \tag{4-27}$$

P and M have disappeared from these equations, so the consistency conditions now involve only the field variables, and not the variables, which are introduced for describing the surface. In fact, these conditions merely say that the p, m shall satisfy Poisson bracket relations corresponding to the operators of translation and rotation in flat space-time. The problem of setting up a relativistic field theory now reduces to finding the quantities p, m to satisfy the Poisson bracket relations (4-25), (4-26), and (4-27).

These quantities, remember, are defined in terms of $K_\perp$ and K_r, the energy density and the momentum

density. The expression for the momentum density is just the same as in curvilinear coordinates. It is determined by geometrical arguments only. Our problem reduces to finding the energy density $K_\perp$ leading to p 's and m 's such that the Poisson bracket relations (4-25), 4-26), and (4-27) are fulfilled.

If we work from a Lorentz-invariant action integral and deduce $K_\perp$ from it by standard Hamiltonian methods, $K_\perp$ will automatically satisfy these requirements in the classical theory. The problem of getting a relativistic quantum theory then reduces the problem of suitably choosing the order of factors which occur in $K_\perp$ so as to satisfy the equations (4-25), (4-26), and (4-27) also in the quantum theory, where the Poisson bracket becomes a commutator and the p, m involve non-commuting quantities.

Let us look at (4-25), (4-26), and (4-27) and substitute for p and m their values in terms of K 's. Then you see that some of these conditions will be independent of $K_\perp$. These are automatically satisfied when we choose K_r properly, in accordance with the geometrical requirements. Some of the conditions are linear in $K_\perp$. These will be satisfied by taking $K_\perp$ to be any three-dimensional scalar density in the space of the x 's. So that there is no problem in satisfying the conditions which are linear in $K_\perp$. The awkward ones to satisfy are the ones which are quadratic in $K_\perp$. They are the following:

$$\left[\int x_r K_\perp d^3x, \int K'_\perp d^3x'\right] = \int K_r d^3x \tag{4-28}$$

(This equation comes from (4-26) where we put $\mu = \perp$, $\rho = r$, and $\sigma = \perp$.)

$$\left[\int x_r K_\perp d^3x, \int x'_s K'_\perp d^3x'\right] = -\int (x_r K_s - x_r K_r)\, d^3x \tag{4-29}$$

(from (427) where we take $\nu = \perp$ and $\sigma = \perp$) So the problem of getting a relativistic quantum field theory now reduces to the problem of finding an energy density $K_\perp$ which satisfies the conditions (428) and (429) when we take into account noncommutation of the factors

We can analyze these conditions a little more when we take into account that the Poisson bracket connecting $K_\perp$ at one point and $K'_\perp$ at another point will be a sum of terms involving delta functions and derivatives of delta functions

$$[K_\perp, K'_\perp] = a\delta + 2b_r\delta_{,r} + c_{rs}\delta_{,rs} + \ldots \tag{4-30}$$

(This delta is the threedimensional delta function in volving the three coordinates x and the three coordinates x' of the first and second points) Here $a = a(x)$, $b = b(x), c = c(x), \ldots$ One could have the coefficients involving also x' ,but then one could replace them by coefficients involving x only at the expense of making some changes in the earlier coefficients in the series There is no fundamental dissymmetry between x and x' , only a dissymmetry in regard to the way the equation is written

(430) is the general relationship connecting the energy density at two pointsNow for many examples, including all the more usual fields,derivatives of the delta function higher than the second do not occurLet us examine this case further

Assume derivatives higher that the second do not occurThat means that the series (430) stops at the

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third termIn this special case we can get quite a bit of information about the coefficients a, b, c by making use of the condition that the Poisson bracket (430) is anti symmetrical between the two points x and x' Inter changing x and x' in (430) ,we get

$$\begin{aligned}[K'_\perp, K_\perp] &= a'\delta - 2b'_r\delta_{,r} + c'_{rs}\delta_{,rs} \\ &= a'\delta - 2\left(b'_r\delta\right)_{,r} + \left(c'_{rs}\delta\right)_{,rs}\end{aligned}$$

(since $\partial b_r\left(x'\right)/\partial x^r = 0$,etc)

$$\begin{aligned}&= a\delta - 2\left(b_r\delta\right)_{,r} + \left(c_{rs}\delta\right)_{,rs} \\ &= \left(a - 2b_{r,r} + c_{rs,rs}\right)\delta + \left(-2b_r + 2c_{rs,r}\right)\delta_{,r} + c_{rs}\delta_{,rs}. \quad (4-31)\end{aligned}$$

The expression (431) must equal minus the expression (430) identicallyIn order that the coefficients of $\delta_{,rs}$ shall agree we must have

$$c_{rs} = 0. \tag{4-32}$$

This then makes the coefficients of $\delta_{,r}$ agreeFinally,in order that the coefficients of δ shall agree,we must have

$$a = b_{r,r} \tag{4-33}$$

This gives us the equation

$$[K_\perp, K'_\perp] = 2b_r\delta_r + b_{r,\gamma}\delta. \tag{4-34}$$

Let us now substitute in (428) and (429) They become

$$\begin{aligned}\int K_r d^3x &= \iint x_r\left(2b_s\delta_{,s} + b_{s,s}\delta\right)d^3x d^3x' \\ &= \int x_r b_{s,s} d^3x \\ &= \int b_r d^3x\end{aligned} \tag{4-35}$$

(Note that $x_{r,s} = \partial x_r/\partial x^s = -\delta_{rs}$)

[79]

$$\begin{aligned}-\int\left(x_r K_s - x_s K_r\right)d^3x &= \iint x_r x'_s\left(2b_t\delta_t + b_{t,t}\delta\right)d^3x d^3x' \\ &= \int\left(-2x_r b_s + x_r x_s b_{t,t}\right)d^3x \\ &= \int\left(-x_r b_s + x_s b_r\right)d^3x\end{aligned} \tag{4-36}$$

This is what our consistency conditions reduce to, and we see that they are satisfied by taking $b_r = K_r$. This is not quite the most general solution; more generally we could have

$$b_r = K_r + \theta_{rs,s} \tag{4-37}$$

for any quantity θ_{rs} satisfying the condition that

$$\int (\theta_{rs} - \theta_{sr})\, d^3x = 0 \tag{4-38}$$

Thus θ can have any symmetrical part and its antisymmetrical part must be a divergence.

That gives the general requirement for a field theory to be relativistic. We have to find the energy density $K_\perp$ satisfying the Poisson bracket relation (4-34) where b_r is connected with the momentum density by (4-37). If we work out the energy density from a Lorentz-invariant action then this condition will certainly be satisfied in the classical theory. It might not be satisfied in the quantum theory because the order of the factors might be wrong. It is only when one can choose the order of the factors in the energy density so as to make (4-34), (4-37) hold accurately that we have a relativistic quantum theory. The conditions which we have here for a quantum theory to be relativistic are less stringent than the ones

which we obtained when we had states defined on general curved surfaces.

I would like to illustrate that by taking the example of Born-Infeld electrodynamics. This is an electrodynamics which is in agreement with Maxwell electrodynamics for weak fields but differs from it for strong fields. (We now refer the electromagnetic field quantities to some absolute unit defined in terms of the charge of the electron and classical radius of the electron, so that we can talk of strong fields and weak fields.) The general equations of the Born-Infeld electrodynamics follow from the action principle:

$$I = \int \sqrt{-\det\left(g_{\mu\nu} + F_{\mu\nu}\right) d^4x} \tag{4-39}$$

We may use curvilinear coordinates at this stage. $g_{\mu\nu}$ gives the metric referred to these curvilinear coordinates and $F_{\mu\nu}$ gives the electromagnetic field referred to the absolute unit.

We can pass from this action integral to a Hamiltonian by using the general procedure. The result is to give us a Hamiltonian in which we have, in addition to the variables needed to describe the surface, the dynamical coordinates $A_r, r = 1, 2, 3$. A_0 turns out to be an unimportant variable just like in the Maxwell field. The conjugate momenta D^r to the A_r are the components of the electric induction, and satisfy the Poisson bracket relations

$$[A_r, D'^s] = g_r^s \delta\left(x - x'\right). \tag{4-40}$$

It turns out that in the Hamiltonian we only have A occurring through its curl, namely through the field quantities:

LECTURES ON QUANTUM MECHANICS

$$B^r = \frac{1}{2}\varepsilon^{rst} F_{st} = \varepsilon^{rst} A_{t,s} \tag{4-41}$$

$\varepsilon^{rst} = 1$ when $(rst) = (1, 2, 3)$ and is anti-symmetrical between the suffixes. The commutation relation between B and D is

$$[B^r, D'^s] = \varepsilon^{rst} \delta_{,t}\left(x - x'\right) \tag{4-42}$$

The momentum density now has the value

$$K_r = F_{rs} D^s \tag{4-43}$$

This is just the same as in the Maxwell theory. It is in agreement with the general principle that the momentum density depends only on geometrical arguments, i.e. on the geometrical character of the fields we are using, and the action principle doesn't matter.

The energy density now has the value

$$K_\perp = \left\{\Gamma^2 - \gamma_{rs}\left(D^r D^s + B^r B^s\right) - \gamma^{rs} F_{rt} F_{su} D^t D^u\right\}^{1/2} \tag{4-44}$$

Here γ_{rs} is the metric in the three-dimensional surface and

$$-\Gamma^2 = \det \gamma_{rs} \tag{4-45}$$

If we work with curved surfaces we require $K_\perp$ to satisfy the Poisson bracket relation (3-31). In the classical theory it must do so because it is deduced from a Lorentz-invariant action integral. But we cannot get it to satisfy the required commutation relationship in the quantum theory. The expression for $K_\perp$ has a square root occurring in it, which makes it very awkward to work with. It seems to be quite hopeless to try to get the commutation relations correctly fulfilled with the coefficients γ^{rs} occurring on the left. So it does not seem to be possible to get a Born-Infeld quantum electro-

dynamics with the state defined on general curved surfaces.

Let us, however, go over to flat surfaces. For that purpose, we need to work out the Poisson bracket relationship (4-34). Now we know that conditions are all right in the classical theory. Classically we must therefore have the Poisson bracket relationship:

$$[K_\perp, K'_\perp] = 2K_r \delta_{,r} + K_{r,r}\delta \tag{4-46}$$

We can see without going into detailed calculations that this must hold also in the quantum theory, because K_r is built up entirely from the quantities D^s and B^t. When we work things out in the quantum theory, we shall have the D 's and the B 's occurring in a certain order, but the D 's and B 's all commute with each other when we take them at the same point. We see that from (4-42). If we put the $x' = x$ we get

$$[B^r, D^s] = \varepsilon^{rst}\delta_{.t}(0) = 0 \tag{4-47}$$

(the derivative of the delta function with the argument 0 is to be taken as zero). Thus we are not bothered by the non-commutation of the D 's and the B 's that occur in K_r. We must therefore get the classical expression, so that the consistency conditions are fulfilled.

So for the Born-Infeld electrodynamics, the consistency conditions for the quantum theory on flat surfaces are fulfilled, while they are not fulfilled on curved surfaces. Physically that means that we can set up the basic equations for a quantum theory of the Born-Infeld electrodynamics agreeing with special relativity, but we should have difficulties if we wanted to have this quantum theory agreeing with general relativity.

That completes the discussion of the consistency

requirements for the quantum theory to be relativistic. However, even if we have satisfied these consistency requirements, we have not yet disposed of all the difficulties. There are some quite formidable difficulties still lying ahead of us. If we were dealing with a system involving only a finite number of degrees of freedom, then we should have disposed of all of the difficulties, and it would be a straightforward matter to solve the differential equations on ψ. But with field theory, we have an infinite number of degrees of freedom, and this infinity may lead to trouble. It usually does lead to trouble.

We have to solve equations in which the unknown, the wave function ψ, involves an infinite number of variables. The usual method that people have for solving this kind of equation is to use perturbation methods in which the wave function is expanded in powers of some small

parameter, and one tries to get a solution step by step. But one usually runs into the difficulty that after a certain stage the equations lead to divergent integrals.

People have done a great deal of work on this problem. They have found methods for handling these divergent integrals which seem to be tolerable to physicists even though they cannot be justified mathematically, and they have built up the renormalization technique, which allows one to disregard the infinities in the case of certain kinds of field theory.

So, even when we have formally satisfied the consistency requirements, we still have the difficulty that we may not know how to get solutions of the wave equation satisfying the required supplementary conditions. If we can get such solutions, there remains the further problem of introducing scalar products for these

[84]

solutions, which means considering these solutions as the vectors in a Hilbert space. It is necessary to introduce these scalar products before we can get a physical interpretation for our wave function in terms of the standard rules for the physical interpretation of quantum mechanics. It is necessary that we should have scalar products for the wave functions which satisfy the supplementary conditions, but we do not need to worry about scalar products for general wave functions which do not satisfy the supplementary conditions. There may be no way of defining scalar products for these general wave functions, but that would not matter at all. The physical interpretation for quantum mechanics requires that scalar products exist only for wave functions satisfying all the supplementary conditions.

You see that there are quite formidable difficulties in getting the Hamiltonian theory to work, in connection with quantum mechanics. So far as concerns classical mechanics, the method seems to be fairly complete and we know exactly what the situation is; but for quantum mechanics we have only really started on the problem. There are the difficulties of finding solutions even when the supplementary conditions are formally consistent, and possibly also the difficulty of introducing scalar products of the solutions.

The difficulties are quite serious, and they have led some physicists to challenge the whole Hamiltonian method. A good many physicists are now working on the problem of trying to set up a quantum field theory independently of any Hamiltonian. Their general method is to introduce quantities which are of physical importance, then to bring in accepted general principles in order to impose conditions on these quantities; and

their hope is that ultimately they will get enough conditions imposed on these quantities of physical importance to be able to calculate them. They are still very far from achieving that end, and my own belief is that it will not be possible to dispense entirely with the Hamiltonian method. The Hamiltonian method dominates mechanics from the classical point of view. It may be that our method of passing from classical mechanics to quantum mechanics is not yet correct. I still think that in any future quantum theory there will have to be something corresponding to Hamiltonian theory, even if it is not in the same form as at present.

I have given the treatment of the Hamiltonian method as far as it has yet been developed. It is quite a general and powerful method which can be adapted to a variety of problems. It can be adapted to problems where singularities (point or surface) occur in the field. The general idea governing this development of the Hamiltonian theory is to find an action I which involves certain parameters q, such that when we vary the q 's, δI is linear in the δq 's. It is indispensable that we should have δI linear in the δq 's in order that we may apply the treatment described in these lectures.

The way to bring about linearity when we have singularities is to work in terms of curvilinear coordinates, and not to vary any equations which determine the position of a singular point or a singular surface. For example, if we are dealing with a singular surface specified by an equation $f(x) = 0$, then we must have a variation principle in which $f(x)$ is not varied. If we

allow $f(x)$ to vary, if we treat f itself as providing some of the q 's, then we do not have δI linear in the δq 's. But we can keep $f(x)$ fixed with respect to some curvilinear

coordinate system x and we can vary the surface by varying the curvilinear coordinate system without varying the function f. Then the general method which I have discussed here works very well in the classical theory. When we go over to quantization we have the difficulties arising which I have discussed.

24.5.6 Introduction to Supersymmetric Quantum Mechanics

(у киселева почитаю, мб выгружу потом, пока не до этого)

24.5.7 Quantum scars

(там крутые картинки есть, похоже на грав волновое линзирование, подумаю потом. все равно много времени нужно, чтобы разобраться.)

Quantum scarring refers to a phenomenon where the eigenstates of a classically chaotic quantum system have enhanced probability density around the paths of unstable classical periodic orbits.[2][3] The instability of the periodic orbit is a decisive point that differentiates quantum scars from the more trivial observation that the probability density is enhanced in the neighborhood of stable periodic orbits. The latter can be understood as a purely classical phenomenon, a manifestation of the Bohr correspondence principle, whereas in the former, quantum interference is essential. As such, scarring is both a visual example of quantum-classical correspondence, and simultaneously an example of a (local) quantum suppression of chaos.

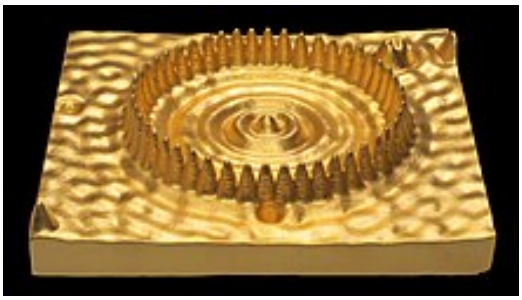
A classically chaotic system is also ergodic, and therefore (almost) all of its trajectories eventually explore evenly the entire accessible phase space. Thus, it would be natural to expect that the eigenstates of the quantum counterpart would fill the quantum phase space in the uniform manner up to random fluctuations in the semiclassical limit. However, scars are a significant correction to this assumption. Scars can therefore be considered as an eigenstate counterpart of how short periodic orbits provide corrections to the universal spectral statistics of the random matrix theory. There are rigorous mathematical theorems on quantum nature of ergodicity,[4][5][6] proving that the expectation value of an operator converges in the semiclassical limit to the corresponding microcanonical classical average. Nonetheless, the quantum ergodicity theorems do not exclude scarring if the quantum phase space volume of the scars gradually vanishes in the semiclassical limit.

24.5.8 Quantum mirage

(там крутые картинки есть, подумаю потом. все равно много времени нужно, чтобы разобраться.)

In physics, a quantum mirage is a peculiar result in quantum chaos. Every system of quantum dynamical billiards will exhibit an effect called scarring, where the quantum probability density shows traces of the paths a classical billiard ball would take. For an elliptical arena, the scarring is particularly pronounced at the foci, as this is the region where many classical trajectories converge. The scars at the foci are colloquially referred to as the "quantum mirage".

The quantum mirage was first experimentally observed by Hari Manoharan, Christopher Lutz and Donald Eigler at the IBM Almaden Research Center in San Jose, California in 2000. The effect is quite remarkable but in general agreement with prior work on the quantum mechanics of dynamical billiards in elliptical arenas.



25 Very Special Methods, Phenomena, Applications

25.1 More on Quantum Scattering Theory

(тут многие другие темы, нпр из ЛЛ3. супер редко они нужны, так что раздел и вдали.)

25.1.1 Gell-Mann and Low theorem

(пока по вики)

Statement of the theorem

Let $|\Psi_0\rangle$ be an eigenstate of H_0 with energy E_0 and let the 'interacting' Hamiltonian be $H = H_0 + gV$, where g is a coupling constant and V the interaction term. We define a Hamiltonian $H_\epsilon = H_0 + e^{-\epsilon|t|}gV$ which effectively interpolates between H and H_0 in the limit $\epsilon \to 0^+$and $|t| \to \infty$. Let $U_{\epsilon I}$ denote the evolution operator in the interaction picture. The Gell-Mann and Low theorem asserts that if the limit as $\epsilon \to 0^+$of

$$\left|\Psi_\epsilon^{(\pm)}\right\rangle = \frac{U_{\epsilon I}(0, \pm\infty)\,|\Psi_0\rangle}{\langle\Psi_0\,|U_{\epsilon I}(0, \pm\infty)|\,\Psi_0\rangle}$$

exists, then $\left|\Psi_\epsilon^{(\pm)}\right\rangle$are eigenstates of H Note that when applied to, say, the ground-state, the theorem does not guarantee that the evolved state will be a ground state. In other words, level crossing is not excluded.

Proof

As in the original paper, the theorem is typically proved making use of Dyson's expansion of the evolution operator. Its validity however extends beyond the scope of perturbation theory as has been demonstrated by Molinari. We follow Molinari's method here. Focus on H_ϵ and let $g = e^{\epsilon\theta}$. From Schrdinger's equation for the time-evolution operator

$$i\hbar\partial_{t_1}U_\epsilon(t_1, t_2) = H_\epsilon(t_1)\,U_\epsilon(t_1, t_2)$$

and the boundary condition $U_\epsilon(t_2, t_2) = 1$ we can formally write

$$U_\epsilon(t_1, t_2) = 1 + \frac{1}{i\hbar}\int_{t_2}^{t_1} dt'\left(H_0 + e^{\epsilon(\theta-|t'|)}V\right)U_\epsilon(t', t_2)$$

Focus for the moment on the case $0 \geq t_1 \geq t_2$. Through a change of variables $\tau = t' + \theta$ we can write

$$U_\epsilon(t_1, t_2) = 1 + \frac{1}{i\hbar}\int_{\theta+t_2}^{\theta+t_1} d\tau\,(H_0 + e^{\epsilon\tau}V)\,U_\epsilon(\tau - \theta, t_2)$$

We therefore have that

$$\partial_\theta U_\epsilon(t_1,t_2) = \epsilon g \partial_g U_\epsilon(t_1,t_2) = \partial_{t_1} U_\epsilon(t_1,t_2) + \partial_{t_2} U_\epsilon(t_1,t_2)$$

This result can be combined with the Schrdinger equation and its adjoint

$$-i\hbar\partial_{t_1} U_\epsilon(t_2,t_1) = U_\epsilon(t_2,t_1) H_\epsilon(t_1)$$

to obtain

$$i\hbar\epsilon g\partial_g U_\epsilon(t_1,t_2) = H_\epsilon(t_1) U_\epsilon(t_1,t_2) - U_\epsilon(t_1,t_2) H_\epsilon(t_2)$$

The corresponding equation between $H_{\epsilon I}, U_{\epsilon I}$ is the same. It can be obtained by pre-multiplying both sides with $e^{iH_0 t_1/\hbar}$, post-multiplying with $e^{iH_0 t_2/\hbar}$ and making use of

$$U_{\epsilon I}(t_1,t_2) = e^{iH_0 t_1/\hbar} U_\epsilon(t_1,t_2) e^{-iH_0 t_2/\hbar}$$

The other case we are interested in, namely $t_2 \geq t_1 \geq 0$ can be treated in an analogous fashion and yields an additional minus sign in front of the commutator (we are not concerned here with the case where $t_{1,2}$ have mixed signs). In summary, we obtain

$$(H_{\epsilon,t=0} - E_0 \pm i\hbar\epsilon g\partial_g) U_{\epsilon I}(0,\pm\infty)|\Psi_0\rangle = 0$$

We proceed for the negative-times case. Abbreviating the various operators for clarity

$$i\hbar\epsilon g\partial_g (U|\Psi_0\rangle) = (H_\epsilon - E_0) U|\Psi_0\rangle$$

Now using the definition of Ψ_ϵ we differentiate and eliminate derivatives $\partial_g(U|\Psi_0\rangle)$ using the above expression, finding

$$\begin{aligned} i\hbar\epsilon g\partial_g|\Psi_\epsilon\rangle &= \frac{1}{\langle\Psi_0|U|\Psi_0\rangle}(H_\epsilon - E_0) U|\Psi_0\rangle - \frac{U|\Psi_0\rangle}{\langle\Psi_0|U|\Psi_0\rangle}\langle\Psi_0|(H_\epsilon - E_0) U|\Psi_0\rangle \\ &= (H_\epsilon - E_0)|\Psi_\epsilon\rangle - |\Psi_\epsilon\rangle\langle\Psi_0|H_\epsilon - E_0|\Psi_\epsilon\rangle \\ &= [H_\epsilon - E]|\Psi_\epsilon\rangle . \end{aligned}$$

where $E = E_0 + \langle\Psi_0|H_\epsilon - H_0|\Psi_\epsilon\rangle$. We can now let $\epsilon \to 0^+$as by assumption the $g\partial_g|\Psi_\epsilon\rangle$ in left hand side is finite. We then clearly see that $|\Psi_\epsilon\rangle$ is an eigenstate of H and the proof is complete.

Примеры применений (???)

(я не знаю, где эта теорема применяется, потому что почти не понял ее. напишу, если узнаю.)

25.1.2 Coulomb Scattering in 4D by Kiselev

(см. его дополнения, это вообще не нужно было, но там очень нетривиальная теория!)

Why does one need it?

(??? I have no idea, I'll think later)

Theory

(???)

25.1.3 More on Scattering Theory

(overview what else is written in books about it)

25.2 Quantum Chemistry

(I think, this is a really important application and I don't know it yet at all)

25.3 Many-Body Quantum Systems

(в статфизе и конд среды целые книги про это, выпишу что-то из них)

фермионы

Для фермионов запишем операторы в матричном представлении:

$$(b)_{m,n} = \delta(m)\delta(n-1), \quad \left(b^\dagger\right)_{m,n} = (b)_{n,m} = \delta(m-1)\delta(n) \quad m,n = 0,1$$

$$b = \begin{bmatrix} 0 & 0.1 \\ 0 & 0 \end{bmatrix}, \quad b^\dagger = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad (c)_{m,n} = (-1)^m\delta(n-m), \quad c = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$bc + cb = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} = 0$$

$$bc + cb = 0, \quad b^\dagger c + cb^\dagger = 0, \quad c^2 = 1$$

$$[bw](n) = \delta(n)w(1), \quad \left[b^\dagger w\right](n) = \delta(n-1)w(0)$$

$$\text{Для вакуумной} w_0 = \delta(n): \quad [bw_0](n) = 0, \quad \left[b^\dagger w_0\right](n) = \delta(n-1)\underset{0.}{w_0}(0) = \delta(n-1)$$

$$\text{Для получается, что } w_1 = \delta(n-1): \quad [bw_1](n) = \delta(n), \quad \left[b^\dagger w_1\right](n) = 0$$

то есть b уменьшает на единицу, $b^\dagger$ - увеличивает.

коммутационные соотношения

$$\begin{gathered} \left[b^\dagger bw\right](n) = [\delta(n-1)\delta(p)\delta(p)\delta(m-1)w(m)](n) = \\ = [\delta(n-1)\delta(m-1)w(m)](n) = nw(n) \\ \left[bb_0^\dagger w\right](n) = [\delta(n)\delta(p-1)\delta(p-1)\delta(m)w(m)](n) = \\ = [\delta(n)\delta(m)w(m)](n) = (1-n)w(n) \\ \left[\left(bb^\dagger + b^\dagger b\right)w\right](n) = w(n), \quad \text{или} \quad bb^\dagger + b^\dagger b = 1 \end{gathered}$$

в матричном виде тоже все видано:

$$b^\dagger b + bb^\dagger = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

осталось проверить, что со степенями операторов
для квадрата:

$$\begin{gathered} [bw](n) = \delta(n)w(1) \to \left[b^2 w\right](n) = 0, b^2 = 0 \\ \left[b^\dagger w\right](n) = \delta(n-1)w(0) \to \left[\left(b^\dagger\right)^2 w\right](n) = 0, \left(b^\dagger\right)^2 = 0 \end{gathered}$$

фермионы продолжение

я вообще хз, просто Кузьмин лекцию читает.

$$\forall w(n): [bw](n) = \delta(n)w(1), \quad \left[b^\dagger w\right](n) = \delta(n-1)w(0)$$
$$w_0(n) = \delta(n): [bw_0](n) = 0, \quad \left[b^\dagger w_0\right](n) = \delta(n-1)$$
$$w_1(n) = \delta(n-1): [bw_1](n) = \delta(n), \quad \left[b^\dagger w_1\right](n) = 0$$
$$\left[\left(bb^\dagger + b^\dagger b\right)w\right](n) = w(n), \quad bb^\dagger + b^\dagger b = 1$$
$$\forall w(n): \quad [b^2 w](n) = 0, b^2 = 0; \quad \left[\left(b^\dagger\right)^2 w\right](n) = 0, \left(b^\dagger\right)^2 = 0.$$

$$\mathcal{C}(...n_f...), \quad n_f = 0, 1$$

$$\forall f: \left(b_f, b_f^\dagger, c_f\right); \quad b_f^2 = 0 = \left(b_f^\dagger\right)^2, \hat{n}_f = b_f^\dagger b_f, b_f b_f^\dagger + b_f^\dagger b_f = 1, b_f c_f + c_f b_f = 0, c_f^2 = 1$$

$\left(b_f, b_f^\dagger, c_f\right)$ действуют на n_f, $\quad \left(b_g, b_g^\dagger, c_g\right)$ действуют на n_g.

При $f \neq g$: операторы действуют независимо.

$b_f b_g - b_g b_f = 0, \quad b_f b_g^\dagger - b_g^\dagger b_f = 0, \quad c_f b_g - b_g c_f = 0, \quad$ (и это называется операторами Паули)

$$\mathcal{C}_{\text{vac}} = \prod_g \delta(n_g), (\mathcal{C}_{\text{vac}}, \mathcal{C}_{\text{vac}}) = 1, b_f \mathcal{C}_{\text{vac}} = 0, b_f^\dagger \mathcal{C}_{\text{vac}} = \delta(n_f - 1) \prod_{g \neq f} \delta(n_f)$$

Операторы Паули и операторы Ферми

Получим операторы B_λ из операторов b, то есть перейдем к другому базису.
делается это с помощью унитарного преобразования.

$$B_\lambda = \sum_f u_{\lambda,f} b_f; \quad \sum_f u_{\lambda,f} u_{\mu,f}^* = \delta(\lambda - \mu), \quad \sum_\lambda u_{\lambda,f} u_{\lambda,g}^* = \delta(g - f)$$

$$B_\lambda B_\lambda^\dagger + B_\lambda^\dagger B_\lambda = \sum_{f,g} u_{\lambda,f} u_{\lambda,g}^* \left(b_f b_g^\dagger + b_g^\dagger b_f\right) =$$
$$= \sum_f u_{\lambda,f} u_{\lambda,f}^* \left(b_f b_f^\dagger + b_f^\dagger b_f\right) + \sum_{f \neq g} u_{\lambda,f} u_{\lambda,g}^* \left(b_f b_g^\dagger + b_g^\dagger b_f\right) =$$
$$= \sum_f u_{\lambda,f} u_{\lambda,f}^* + \sum_{f \neq g} u_{\lambda,f} u_{\lambda,g}^* \left(b_f b_g^\dagger + b_g^\dagger b_f\right) = 1 + \sum_{f \neq g} u_{\lambda,f} u_{\lambda,g}^* \left(b_f b_g^\dagger + b_g^\dagger b_f\right)$$

И у нас чтобы был ноль, то есть преобразование было унитарным, нужно, чтобы в правой части занулялось кое-что.

Перестановочные соотношения для операторов Паули не сохраняются при унитарных преобразованиях!

Вводим операторы с помощью домножения на операторы c

$$a_f \equiv \left(\prod_{g<f} c_g\right) b_f = b_f \left(\prod_{g<f} c_g\right) \quad (c_g b_f = b_f c_g, g \neq f);$$

и можем спокойно создать эрмитово сопряженный

$$a_f^\dagger = \left(\prod_{g<f} c_g\right) b_f^\dagger$$

при этому конструкция такова, что основные соотношения не поменялись, действительно:

$$a_f^\dagger a_f = \left(\prod_{g<f} c_g\right) b_f^\dagger \left(\prod_{h<f} c_h\right) b_f = \left(\prod_{g<f} c_g\right)\left(\prod_{h<f} c_h\right) b_f^\dagger b_f = b_f^\dagger b_f = \hat{n}_f$$

и также:

$$a_f^2 = \left(a_f^\dagger\right)^2 = 0, \quad a_f a_f^\dagger + a_f^\dagger a_f = b_f b_f^\dagger + b_f^\dagger b_f = 1$$

теперь посмотрим что мы получили:

$$f < g: \quad a_f a_g + a_g a_f = \left(\prod_{h<f} c_h\right) b_f \left(\prod_{i<g} c_i\right) b_g + \left(\prod_{i<g} c_i\right) b_g \left(\prod_{h<f} c_h\right) b_f \neq \Bigg)$$

$$= b_f \left(\prod_{h<f} c_h\right)\left(\prod_{i<g} c_i\right) b_g + b_g \left(\prod_{i<g} c_i\right)\left(\prod_{h<f} c_h\right) b_f = b_f \left(\prod_{f\le i<g} c_i\right) b_g + b_g \left(\prod_{f\le h<g} c_h\right) b_f =$$

но тепер ь операторов i больше, чем операторов h

но один из операторов c будет антикоммутировать с b, так что вынесется все так:

$$= b_f b_g \left(\prod_{f\le i<g} c_i\right) - b_g b_f \left(\prod_{f\le h<g} c_h\right) = [b_f b_g - b_g b_f]\left(\prod_{f\le h<g} c_h\right) = 0$$

в последнем равенстве у нас появились операторы паули, коммутатор который равен нулю.

и имеем:

$$c_g^\dagger = c_g, \quad f < g: \quad a_f a_g^\dagger + a_g^\dagger a_f = 0$$

а поскольку все симметрично, то можно сказать, что так для любого:

$$\forall f, g: \quad a_f a_g + a_g a_f = 0, \quad a_f a_g^\dagger + a_g^\dagger a_f = \delta(g - f)$$

и именно из-за этой конструкции это называется операторами ферми.

таким образом, они выживают при унитарном преобразовании

и строго говоря они не являются одночастичными операторами, потому что есть в них часть, которая действует на все частицы.

в квантовой механике операторы, которые действуют на разные координаты коммутрируют, поэтому операторы Паули коммутируют, но они не обладают унитарностью, поэтому вводятся операторы, которые похожие на одночастичные, но по факту они многочастинчые. и они антикоммутируют, а не коммутируют.

и казалось бы, что операторы действуют на разные части системы и антикоммутируют.

секрет в том, что есть члены, которые действуют на другие части системы

получили операторы Ферми

$$B_\lambda = \sum_f u_{\lambda,f} a_f, \sum_f u_{\lambda,f} u_{\mu,f}^* = \delta(\lambda - \mu), \quad B_\lambda B_\mu^\dagger + B_\mu^\dagger B_\lambda = \delta(\mu - \lambda)$$

$$[cw](n) = (-1)^n w_n \to c_f \mathcal{C}_{\text{vac}} = \mathcal{C}_{\text{vac}};$$

поэтому когда действуем на вакуум, делается это так:

$$a_f \mathcal{C}_{\text{vac}} = b_f \prod_{h<f} c_h \mathcal{C}_{\text{vac}} = b_f \mathcal{C}_{\text{vac}} = 0$$

$$a_f^\dagger \mathcal{C}_{\text{vac}} = b_f \prod_{h<f} c_h \mathcal{C}_{\text{vac}} = b_f^\dagger \mathcal{C}_{\text{vac}} = \delta(n_f - 1) \prod_{g \neq f} \delta(n_g)$$

$$g < f: \quad a_g^\dagger a_f^\dagger \mathcal{C}_{\text{vac}} = b_g^\dagger \left(\prod_{h<g} c_h \right) \delta(n_f - 1) \prod_{k \neq f} \delta(n_k) = \delta(n_f - 1)\, \delta(n_g - 1) \prod_{k \neq g,f} \delta(n_k)$$

теперь давайте посмотрим, чему равен оператор:

$$a_{g_1}^\dagger a_{g_2}^\dagger ... a_{g_N}^\dagger \mathcal{C}_{\text{vac}} = \delta(n_{g_1} - 1)\, \delta(n_{g_2} - 1) ... \delta(n_{g_n} - 1) \prod_{f \neq g_1 ... g_N} \delta(n_f)$$

где

$$g_1 < g_2 < ... < g_N :$$

рассмотрим

$$\frac{1}{\sqrt{N!}} \sum_{f_1,...,f_N} F(f_1, ... f_N)\, a_{f_1}^\dagger ... a_{f_N}^\dagger \mathcal{C}_{\text{vac}} =$$

$$= \frac{1}{\sqrt{N!}} \sum_{\substack{(...m_f...) \\ \sum_f m_f = N}} \sum_{\substack{f_1,...,f_f \\ (...m_f \cdots)}} F(f_1, ..., f_N)\, a_{f_1}^\dagger ... a_{f_N}^\dagger \mathcal{C}_{\text{vac}}$$

$$\sum_{\substack{f_1,...,f_N \propto \\ (...m_f \cdots)}} F(f_1, ..., f_N)\, a_{f_1}^\dagger ... a_{f_N}^\dagger \mathcal{C}_{\text{vac}} =$$

$$= N! F(g_1, ..., g_N)\, a_{g_1}^\dagger ... a_{g_N}^\dagger \mathcal{C}_{\text{vac}}, \quad (g_1 < g_2 < ... < g_N);$$

$$\frac{1}{\sqrt{N!}} \sum_{f_1,...,f_N} F(f_1, ... f_N)\, a_{f_1}^\dagger ... a_{f_N}^\dagger \mathcal{C}_{\text{vac}} =$$

$$= \sqrt{N!} \sum_{\substack{(...m_f...) \\ \sum_f m_f = N}} F(g_1, ..., g_N)\, a_{g_1}^\dagger ... a_{g_N}^\dagger \mathcal{C}_{\text{vac}}$$

таким образом, это сумма по всем числам заполнений.
потому что они образуют базис и можно разложить по нему
????
Волновая функция в пространстве чисел заполнения

$$a_{g_1}^\dagger a_{g_2}^\dagger ... a_{g_N}^\dagger \mathcal{C}_{\text{vac}} = \prod_g \delta(n_g - m_g)$$

где $m_g = 0$, если $g \neq g_1, g_2, ... g_N$; $m_g = 1$, если $g = g_k, k = 1, 2 ... N$
Определение: $\mathcal{C}(...n_f...) = \sqrt{N!} F(g_1, ..., g_N)$, где $(g_1 < g_2 < ... < g_N)(...n_f...)$
это амплитуда вероятности нахождения именно в этой состоянии чисел заполнения.

$$\frac{1}{\sqrt{N!}}\sum_{f_1,...,f_N} F\left(f_1,...f_N\right) a^\dagger_{f_1}...a^\dagger_{f_N}\mathcal{C}_{\text{vac}} =$$
$$\sum_{(...m_f...)} \mathcal{C}\left(...m_f...\right)\left\{\prod_g \delta\left(n_g - m_g\right)\right\} =$$
$$\sum_f m_f = N$$
$$= \mathcal{C}\left(...n_f...\right)$$

Для фермионов

$$\mathcal{C} = \frac{1}{\sqrt{N!}}\sum_{f_1,...,f_N} F\left(f_1,...f_N\right) a^\dagger_{f_1}...a^\dagger_{f_N}\mathcal{C}_{\text{vac}}$$

таким образом, мы получили функцию в пространстве чисел заполнения.

в итоге формула одна и та же, но смысл элементов в этой формуле разный для бозонов и фермионов.

Бозоны	Фермионы
$F\left(f_1,...,f_N\right)$ - симметричная	$F\left(f_1,...,f_N\right)$ - антисимметричная
$n_f = 0,1,...,N$	$n_f = 0,1$
$a_f a^\dagger_g - a^\dagger_g a_f = \delta(g-f)$	$a_f a^\dagger_g + a^\dagger_g a_f = \delta(g-f)$
$a_f a_g - a_g a_f = 0$	$a_f a_g + a_g a_f = 0$
$a^\dagger_f a^\dagger_g - a^\dagger_g a^\dagger_f = 0$	$a^\dagger_f a^\dagger_g + a^\dagger_g a^\dagger_f = 0$
Вакуумная волновая функция $a_f\mathcal{C}_{\text{vac}} = 0$	

для бозонов - операторы коммутируют, для фермионов - антикоммутируют.

и в обоих случаях вакуумное состояние опередеяется с помощью действия A_f

фоковское представление

$$\mathcal{C} = \frac{1}{\sqrt{N!}}\sum_{f_1,...,f_N} F\left(f_1,...f_N\right) a^\dagger_{f_1}...a^\dagger_{f_N}\mathcal{C}_{\text{vac}}$$

$$F\left(f_1,...f_N\right) = \int \varphi\left(x_1,...,x_N\right)\psi^*_{f_1}\left(x_1\right)...\psi^*_{f_N}\left(x_N\right)dx_1...dx_N$$

$$\mathcal{C} = \frac{1}{\sqrt{N!}}\sum_{f_1,...,f_N}\int \varphi\left(x_1,x_2,...,x_N\right)\psi^*_{f_1}\left(x_1\right)\psi^*_{f_2}\left(x_2\right)...\psi^*_{f_N}\left(x_N\right)dx_1dx_2...dx_N\times$$
$$\times a^\dagger_{f_1}a^\dagger_{f_2}...a^\dagger_{f_N}\mathcal{C}_{\text{vac}}$$

введем функции, зависящие от координат вида

$$\Psi^\dagger(x) \equiv \sum_f \psi^*_f(x)a^\dagger_f, \quad \Psi(x) = \sum_f \psi_f(x)a_f$$

через эти функции можно записать волновую функцию в пространстве чисел заполнения:

сумма уходит после перехода к Ψ

$$\mathcal{C} = \frac{1}{\sqrt{N!}}\int \varphi\left(x_1,x_2,...,x_N\right)\Psi^\dagger\left(x_1\right)\Psi^\dagger\left(x_2\right)...\Psi^\dagger\left(x_N\right)dx_1dx_2...dx_N\mathcal{C}_{\text{vac}}$$

эта конструкция называется представлением фока или функционалом Фока.

$$\text{Для всех } x: \Psi(x)\mathcal{C}_{\text{vac}} = 0; \quad (\mathcal{C}_{\text{vac}}, \mathcal{C}_{\text{vac}}) = 1.$$

коммутационные соотношения

$$[A, B]_{\pm} \equiv AB \pm BA$$

$$\left[a_f, a_g^{\dagger}\right]_{\pm} = a_f a_g^{\dagger} \pm a_g^{\dagger} a_f = \delta\left(f^{0\cdot} g\right), \quad [a_f, a_g]_{\pm} = a_f a_g \pm a_g a_f = 0$$

знак " + " для фермионов и знак " - " для бозонов.
Дальше посмотрим на

$$\left[\Psi(x), \Psi^{\dagger}(y)\right]_{\pm} = \Psi(x)\Psi^{\dagger}(y) \pm \Psi^{\dagger}(y)\Psi(x) =$$

и дальше выносим операторы, по соотношению полноты появляется дельта функция и по соотношению полноты приходим к дельта функции.

$$= \sum_{f,g} \left[\psi_f(x) a_f, \psi_g^*(y) a_g^{\dagger}\right]_{\pm} = \sum_{f,g} \psi_f(x)\psi_g^*(y) \left[a_f, a_g^{\dagger}\right]_{\pm} = \sum_{f,g} \psi_f(x)\psi_g^*(y)\delta(g-f) =$$

$$= \sum_{f} \psi_f(x)\psi_f^*(y) = \delta(f-g)$$

здесь знак + для фермионов, - для бозонов
Аналогично,

$$[\Psi(x), \Psi(y)]_{\pm} = 0$$

$\Psi(x)$ - будет нужна позже для...

Вторичное квантование по Кузьмину 2

кузьмин лекция 12 наверное, просто выгрузка
$\Psi(y) \int \Psi^{\dagger}(x_1) ... \Psi^{\dagger}(x_N) \mathcal{C}_{\text{vac}} \varphi(x_1, ... x_N)\, dx_1 ... dx_N = ?$
Введем $T_{j_1, j_2} : x_{j_1} \to x_{j_2}, x_{j_2} \to x_{j_1}, j_1 \neq j_2; T_{j_1,j_2}\varphi(x_1, ... x_N) = \varepsilon\varphi(x_1, ... x_N)$
$\Psi(y)\Psi^{\dagger}(x_1) ... \Psi^{\dagger}(x_N)\mathcal{C}_{\text{vac}} = \left\{\Psi(y)\Psi^{\dagger}(x_1) = \delta(x_1 - y) + \varepsilon\Psi^{\dagger}(x_1)\Psi(y)\right\} =$
$= \delta(x_1 - y)\Psi^{\dagger}(x_2) ... \Psi^{\dagger}(x_N)\mathcal{C}_{\text{vac}} + \varepsilon\Psi^{\dagger}(x_1)\Psi(y)\Psi^{\dagger}(x_2) ... \Psi^{\dagger}(x_N)\mathcal{C}_{\text{vac}} =$
$= \delta(x_1 - y)\Psi^{\dagger}(x_2) ... \Psi^{\dagger}(x_N)\mathcal{C}_{\text{vac}} + \varepsilon\delta(x_2 - y)\Psi^{\dagger}(x_1)\Psi^{\dagger}(x_3) ... \Psi^{\dagger}(x_N)\mathcal{C}_{\text{vac}} +$
$+\varepsilon^2\Psi^{\dagger}(x_1)\Psi^{\dagger}(x_2)\Psi(y)\Psi^{\dagger}(x_3) ... \Psi^{\dagger}(x_N)\mathcal{C}_{\text{vac}} = = \{$ до тех пор, пока не получим $\Psi^{\dagger}(x_1)\Psi^{\dagger}(x_2) ... \Psi^{\dagger}(x_N)\Psi(y)\mathcal{C}_{\text{vac}} = 0\} =$
$\left[\Psi^{\dagger}(x_1) ... \Psi^{\dagger}(x_N)\right]_j \equiv \Psi^{\dagger}(x_1) ... \Psi^{\dagger}(x_{j-1}) 1 \Psi^{\dagger}(x_{j+1}) ... \Psi^{\dagger}(x_N)$ в каждом $\left[\Psi^{\dagger}(x_1) ... \Psi^{\dagger}(x_N)\right]_j$ x_1 на j -ое место: $\left[\Psi^{\dagger}(x_1) ... \Psi^{\dagger}(x_N)\right]_j = \varepsilon^{j-2}\left[\Psi^{\dagger}(x_2) ... \Psi^{\dagger}(x_N)\right]_{x_j \to x_1}$
$\Psi(y)\Psi^{\dagger}(x_1) ... \Psi^{\dagger}(x_N)\mathcal{C}_{\text{vac}} = \delta(x_1 - y)\Psi^{\dagger}(x_2) ... \Psi^{\dagger}(x_N)\mathcal{C}_{\text{vac}} +$
$+ \sum_{j=2}^{N} \varepsilon^{j-1}\varepsilon^{j-2} T_{1,j}\left[\delta(x_1 - y)\Psi^{\dagger}(x_2) ... \Psi^{\dagger}(x_N)\right]\mathcal{C}_{\text{vac}}; \quad \varepsilon^{j-1}\varepsilon^{j-2} = \varepsilon$
$\int \Psi(y)\Psi^{\dagger}(x_1) ... \Psi^{\dagger}(x_N)\mathcal{C}_{\text{vac}}\varphi(x_1, ... x_N)\, dx_1 ... x_N =$
$= \int \delta(x_1 - y)\Psi^{\dagger}(x_2) ... \Psi^{\dagger}(x_N)\mathcal{C}_{\text{vac}}\varphi(x_1, ... x_N)\, dx_1 ... x_N +$
$+ \sum_{j=2}^{N} \varepsilon \int T_{1,j}\left[\delta(x_1 - y)\Psi^{\dagger}(x_2) ... \Psi^{\dagger}(x_N)\right]\mathcal{C}_{\text{vac}}\varphi(x_1, ... x_N)\, dx_1 ... x_N$ в сумме по j в каждом слагаемом замена переменных $x_1 \to x_j$:
$\varepsilon \int T_{1,j}\left[\delta(x_1 - y)\Psi^{\dagger}(x_2) ... \Psi^{\dagger}(x_N)\right]\mathcal{C}_{\text{vac}}\varphi(x_1, ... x_N)\, dx_1 ... x_N =$

$$= \varepsilon \int \left[\delta(x_j - y)\,\Psi^\dagger(x_2)\,...\Psi^\dagger(x_N)\right] \mathcal{C}_{\text{vac}} T_{1,j}\varphi(x_1,...x_N)\,dx_1...x_N =$$
$$= \int \delta(x_1 - y)\,\Psi^\dagger(x_2)\,...\Psi^\dagger(x_N)\,\mathcal{C}_{\text{vac}}\varphi(x_1,...x_N)\,dx_1...x_N$$

Итог: $\int \Psi(y)\Psi^\dagger(x_1)\,...\Psi^\dagger(x_N)\,\mathcal{C}_{\text{vac}}\,\varphi(x_1,...x_N)\,dx_1...x_N =$
$$= N\int \Psi^\dagger(x_2)\,...\Psi^\dagger(x_N)\,\mathcal{C}_{\text{vac}}\,\delta(x_1 - y)\,\varphi(x_1,...x_N)\,dx_1...x_N$$

$\int \Psi(y_2)\,\Psi(y_1)\,\Psi^\dagger(x_1)\,...\Psi^\dagger(x_N)\,\mathcal{C}_{\text{vac}}\varphi(x_1,...x_N)\,dx_1...x_N =$
$$= N\int \Psi(y_2)\,\Psi^\dagger(x_2)\,...\Psi^\dagger(x_N)\,\mathcal{C}_{\text{vac}}\delta(x_1 - y_1)\,\varphi(x_1,...x_N)\,dx_1...x_N =$$
$$= N(N-1)\int \Psi^\dagger(x_3)\,...\Psi^\dagger(x_N)\,\mathcal{C}_{\text{vac}}\delta(x_1 - y_1)\,\delta(x_2 - y_2)\,\varphi(x_1,...x_N)\,dx_1...x_N$$

$$\int \Psi(y_N)\,\Psi(y_{N-1})\,...\Psi(y_1)\,\Psi^\dagger(x_1)\,...\Psi^\dagger(x_N)\,\mathcal{C}_{\text{vac}}\varphi(x_1,...x_N)\,dx_1...x_N =$$
$$= N!\int \mathcal{C}_{\text{vac}}\delta(x_1 - y_1)\,...\delta(x_N - y_N)\,\varphi(x_1,...x_N)\,dx_1...x_N$$

Некоторые произведения

$$\int \left(\mathcal{C}_{\text{vac}}, \Psi(y_N)\,\Psi(y_{N-1})\,...\Psi(y_1)\,\Psi^\dagger(x_1)\,...\Psi^\dagger(x_N)\,\mathcal{C}_{\text{vac}}\right)\varphi(x_1,...x_N)\,dx_1...x_N$$
$$= N!\int (\mathcal{C}_{\text{vac}}, \mathcal{C}_{\text{vac}})\,\delta(x_1 - y_1)\,...\delta(x_N - y_N)\,\varphi(x_1,...x_N)\,dx_1...x_N =$$
$$= N!\varphi(y_1,...y_N)$$

Среднее от произведения $(\Phi, AB\Phi) = \left(A^\dagger\Phi, B\Phi\right)$

$$\int \left(\Psi^\dagger(y_1)\,...\Psi^\dagger(y_N)\,\mathcal{C}_{\text{vac}}, \Psi^\dagger(x_1)\,...\Psi^\dagger(x_N)\,\mathcal{C}_{\text{vac}}\right)\varphi(x_1,...x_N)\,dx_1...x_N =$$
$$= N!\varphi(y_1,...y_N)$$

$$(\mathcal{C}_{\text{vac}}, \Psi(y_N)\,...\Psi(y_1)\,\mathcal{C}) =$$
$$\tfrac{1}{N!}\int \left(\mathcal{C}_{\text{vac}}, \Psi(y_N)\,...\Psi(y_1)\,\Psi^\dagger(x_1)\,...\Psi^\dagger(x_N)\,\mathcal{C}_{\text{vac}}\right)\varphi(x_1,...x_N)\,dx_1...x_N =$$
$$= \sqrt{N!}\varphi(y_1,...y_N)$$

Прямое и обратное преобразования

$$\mathcal{C} = \tfrac{1}{\sqrt{N!}}\int \varphi(x_1,...,x_N)\,\Psi^\dagger(x_1)\,...\Psi^\dagger(x_N)\,\mathcal{C}_{\text{vac}}dx_1...dx_N$$
$$\varphi(x_1,...,x_N) = \tfrac{1}{\sqrt{N!}}\left(\mathcal{C}_{\text{vac}}, \Psi(x_N)\,...\Psi(x_1)\,\mathcal{C}\right)$$

По $\varphi(x_1,...,x_N)$ вычислили $\mathcal{C}\{\varphi\}$, и по $\mathcal{C}$ вычислили $\varphi\{\mathcal{C}\}$.

$$\varphi_1 \to \mathcal{C}_1 = \mathcal{C}\{\varphi_1\}, \quad \varphi_2 \to \mathcal{C}_2 = \mathcal{C}\{\varphi_2\}$$

$$(\mathcal{C}_1, \mathcal{C}_2) = \frac{1}{N!}\int \varphi_1^*(x_1,...,x_N)\,\varphi_2(y_1,...,y_N)\times$$

$$\varphi_1 \to \mathcal{C}_1 = \mathcal{C}\{\varphi_1\}, \quad \varphi_2 \to \mathcal{C}_2 = \mathcal{C}\{\varphi_2\}$$
$$(\mathcal{C}_d, \mathcal{C}_2) = \tfrac{1}{N!}\int \varphi_1^*(x_1,...,x_N)\,\varphi_2(y_1,...,y_N)\times$$
$$\times\left(\Psi^\dagger(x_1)\,...\Psi^\dagger(x_N)\,\mathcal{C}_{\text{vac}}, \Psi^\dagger(y_1)\,...\Psi^\dagger(y_N)\,\mathcal{C}_{\text{vac}}\right)dy_1...dy_N dx_1...dx_N =$$

$$= \tfrac{1}{N!}N!\int \varphi_1^*(x_1,...,x_N)\,\varphi_2(y_1,...,y_N)\times$$
$$\times\delta(y_1 - x_1)\,...\delta(y_N - x_N)\,dy_1...dy_N dx_1...dx_N = (\varphi_1, \varphi_2)$$

Операторы Определяющее условие: $(\varphi_1, D\varphi) = (\mathcal{C}_1, \mathbf{D}\mathcal{C}), \quad \mathcal{C} = \mathcal{C}\{\varphi\}, \mathcal{C}_1 = \mathcal{C}\{\varphi_1\}$

$$\varphi(x_1,...,x_N) \to \mathcal{C} = \mathcal{C}\{\varphi\}, \quad D\varphi \to \mathcal{C}' = \mathcal{C}\{D\varphi\}, \quad \mathbf{D} : \mathcal{C}' = \mathbf{D}\mathcal{C}$$

$\forall\varphi_1(x_1,...,x_N) : (\varphi_1, D\varphi) = (\mathcal{C}_1, \mathcal{C}')$ (сохранение скалярного произведения) Аддитивный оператор

$$\mathfrak{A} = \sum_{j=1}^{N} A_j; \quad \mathcal{C}' = \mathcal{C}\{\mathfrak{A}\varphi\} =$$

$$= \frac{1}{\sqrt{N!}} \int \Psi^{\dagger}(x_1) ... \Psi^{\dagger}(x_N) \mathcal{C}_{\text{vac}}[\mathfrak{A}\varphi](x_1, ..., x_N) \, dx_1 ... dx_N =$$
$$= \frac{N}{\sqrt{N!}} \int \Psi^{\dagger}(x_1) ... \Psi^{\dagger}(x_N) \mathcal{C}_{\text{vac}} A(x_1, y) \varphi(y, x_2, ..., x_N) \, dy dx_1 dx_2 ... dx_N =$$
$$= \frac{N}{\sqrt{N!}} \int \Psi^{\dagger}(x) A(x, y) \Psi^{\dagger}(x_2) ... \Psi^{\dagger}(x_N) \mathcal{C}_{\text{vac}} \varphi(y, x_2 ..., x_N) \, dx_2 ... dx_N dx dy$$

Слайд 6: $N \int \Psi^{\dagger}(x_2) ... \Psi^{\dagger}(x_N) \mathcal{C}_{\text{vac}} \varphi(y, x_2 ..., x_N) \, dx_2 ... dx_N =$
$= \int \Psi(y) \Psi^{\dagger}(x) \Psi^{\dagger}(x_2) ... \Psi^{\dagger}(x_N) \mathcal{C}_{\text{vac}} \varphi(x, x_2, ..., x_N) \, dx dx_2 ... dx_N$

$$\mathcal{C}' = \mathcal{C}\{\mathfrak{A}\varphi\} = \frac{1}{\sqrt{N!}} \int\limits_{\nvdash} \Psi^{\dagger}(x) A(x, y) \Psi(y) dx dy \times$$
$$\times \int \Psi^{\dagger}(x_1) ... \Psi^{\dagger}(x_N) \mathcal{C}_{\text{vac}} \varphi(x_1, ..., x_N) \, dx_1 ... dx_N = \int \Psi^{\dagger}(x) A(x, y) \Psi(y) dx dy \mathcal{C}$$
$$\mathbf{A} = \int \Psi^{\dagger}(x) A(x, y) \Psi(y) dy dx = \int \Psi^{\dagger}(x) [A\Psi](x) dx$$

Плотность числа частиц: $r(\vec{q}) = \sum\limits_{j=1}^{N} \delta(\vec{q} - \vec{q}_j)$; $[r\Psi](\vec{q}_1, \nu) = \delta(\vec{q} - \vec{q}_1) \Psi(\vec{q}_1, \nu)$ $\mathbf{r}(\vec{q}) =$
$\sum\limits_{\nu} \int \Psi^{\dagger}(\vec{q}_1, \nu) \delta(\vec{q} - \vec{q}_1) \Psi(\vec{q}_1, \nu) \, d\vec{q}_1 = \sum\limits_{\nu} \Psi^{\dagger}(\vec{q}, \nu) \Psi(\vec{q}, \nu)$

Число частиц: $\mathbf{N} = \int \mathbf{r}(\vec{q}) d\vec{q} = \sum\limits_{\nu} \int \Psi^{\dagger}(\vec{q}, \nu) \Psi(\vec{q}, \nu) d\vec{q} = \int \Psi^{\dagger}(x) \Psi(x) dx = \sum\limits_{f} a_f^{\dagger} a_f$

для

$$\mathcal{C} = \frac{1}{\sqrt{N!}} \int \varphi(x_1, ..., x_N) \Psi^{\dagger}(x_1) ... \Psi^{\dagger}(x_N) \mathcal{C}_{\text{vac}} dx_1 ... dx_N$$
$$(\mathbf{N} - N)\mathcal{C} = 0; \quad \mathbf{N}\Psi(x)\mathcal{C} = (N-1)\Psi(x)\mathcal{C}; \quad \mathbf{N}\Psi^{\dagger}(x)\mathcal{C} = (N+1)\Psi^{\dagger}(x)\mathcal{C}$$

оператор для взаимодействия двух частиц

$$\mathfrak{B} \equiv \sum_{1 \le j_1 < j_2 \le N} B_{j_1, j_2} = \frac{1}{2} \sum_{1 \le j_1, j_2 \le N; j_1 \ne j_2} B_{j_1, j_2}$$
Лекция 8: $\int \Theta(X) [\mathfrak{B}\Phi](X) dX = \frac{N(N-1)}{2} \int \Theta(x_1, x_2, x_3, ..., x_N) \times$
$\times B(x_1, x_2; y_2, y_1) \Phi(y_1, y_2, x_3, ..., x_N) \, dy_1 dy_2 dx_1 dx_2 ... dx_N$

то есть перестановочная симметрия от такого оператора сводится к большому числу одинаковых интегралов.

Ну и просто действуем этим оператором и считаем функционал Фока от этой конструкции.

Выпишем по сути оперделеение функционала для данного случая:

$$\mathcal{C}\{\mathfrak{B}\varphi\} = \frac{1}{\sqrt{N!}} \int \Psi^{\dagger}(x_1) ... \Psi^{\dagger}(x_N) \mathcal{C}_{\text{vac}} [\mathfrak{B}\varphi](x_1, ..., x_N) \, dx_1 ... dx_N =$$

$$= \frac{N(N-1)}{2} \frac{1}{\sqrt{N!}} \int \Psi^{\dagger}(x_1) \Psi^{\dagger}(x_2) \Psi^{\dagger}(x_3) ... \Psi^{\dagger}(x_N) \mathcal{C}_{\text{vac}} B(x_1, x_2; y_2, y_1) \times$$
$$\times \varphi(y_1, y_2, x_3 ..., x_N) \, dy_1 dy_2 dx_1 dx_2 ... dx_N$$

такие уже интегралы у нас возникали про дейсвтии функционала фока...

только у нас число действий операторов больше, так как у нас теперь двухчастичный оператор.

а мы уже заметили, что

$$N(N-1) \int \Psi^{\dagger}(x_3) ... \Psi^{\dagger}(x_N) \mathcal{C}_{\text{vac}} \varphi(y_1, y_2, x_3, ..., x_N) \, dx_3 ... dx_N =$$
$$= \int \Psi(y_2) \Psi(y_1) \Psi^{\dagger}(x_1) \Psi^{\dagger}(x_2) ... \Psi^{\dagger}(x_N) \mathcal{C}_{\text{vac}} \varphi(x_1, x_2, ..., x_N) \, dx_1 dx_2 ... dx_N$$

то есть у нас функционал фока и два оператора умножения.

$$\mathcal{C}\{\mathfrak{B}\varphi\} = \frac{1}{2}\int \Psi^{\dagger}(x_1)\,\Psi^{\dagger}(x_2)\,B(x_1,x_2;y_2,y_1)\,\Psi(y_2)\,\Psi(y_1)\,dy_1dy_2dx_1dx_2\mathcal{C}\{\varphi\}$$

в итоге симметричный двухчастичный оператор равен

$$\begin{gathered}\mathbf{B} = \tfrac{1}{2}\int \Psi^{\dagger}(x_1)\,\Psi^{\dagger}(x_2)\,B(x_1,x_2;y_2,y_1)\,\Psi(y_2)\,\Psi(y_1)\,dy_1dy_2dx_1dx_2 = \\ = \tfrac{1}{2}\int \Psi^{\dagger}(x_1)\,\Psi^{\dagger}(x_2)\,[B_{1,2}\Psi_2\Psi_1](x_1,x_2)\,dx_1dx_2\end{gathered}$$

$$\begin{gathered}\text{Iror: } \int \Psi(y)\Psi^{\dagger}(x_1)\ldots\Psi^{\dagger}(x_N)\,\mathcal{C}_{\text{vac}}\,\varphi(x_1,\ldots x_N)\,dx_1\ldots x_N = \\ = N\int \Psi^{\dagger}(x_2)\ldots\Psi^{\dagger}(x_N)\,\mathcal{C}_{\text{vac}}\,\delta(x_1-y)\,\varphi(x_1,\ldots x_N)\,dx_1\ldots x_N \\ \int \Psi(y_2)\,\Psi(y_1)\,\Psi^{\dagger}(x_1)\ldots\mathscr{U}^{\dagger}(x_N)\,\mathcal{C}_{\text{vac}}\,\varphi(x_1,\ldots x_N)\,dx_1\ldots x_N = \\ = N\int \Psi(y_2)\,\Psi^{\dagger}(x_2)\ldots\Psi^{\dagger}(x_N)\,\mathcal{C}_{\text{vac}}\,\delta(x_1-y_1)\,\varphi(x_1,\ldots x_N)\,dx_1\ldots x_N = \\ = N!\int \mathcal{C}_{\text{vac}}\,\delta(x_1-y_1)\ldots\delta(x_N-y_N)\,\varphi(x_1,\ldots x_N)\,dx_1\ldots x_N\end{gathered}$$

гамильтониан

(13я лекция кузьмина)

$$\begin{gathered}H = \sum_{1\le J\le N} T_j + \sum_{1\le j_1<j_2\le N} U_{j_1,j_2} \\ T^*(x,y) = T(y,x), \quad U^*(x_1,x_2;y_2,y_1) = U(y_1,y_2;x_2,x_1) \\ H = -\sum_{1\le J\le N}\frac{\hbar^2}{2m}\Delta_{q_j} + \sum_{1\le j_1<j_2\le N} V(q_{j_1}-q_{j_2}), \quad V(-q) = V(q) \\ T(x,x') = -\frac{\hbar^2}{2m}\Delta_q\delta(x'-x) = -\frac{\hbar^2}{2m}\Delta_q\delta(q'-q)\,\delta(\nu'-\nu) \\ U(x_1,x_2;x_2',x_1') = V(q_2-q_1)\,\delta(q_1'-q_1)\,\delta(q_2'-q_2)\,\delta(\nu_1'-\nu_1)\,\delta(\nu_2'-\nu_2).\end{gathered}$$

гамильтониан теперь во вторично квантованном представлении не зависит от числа частиц!

и он одинаков для фермионов и бозонов

$$\begin{gathered}\mathbf{H} = -\tfrac{\hbar^2}{2m}\int \Psi^{\dagger}(x)\Delta_q\Psi(x)dx + \\ +\tfrac{1}{2}\iint V(q_1-q_2)\,\Psi^{\dagger}(x_1)\,\Psi^{\dagger}(x_2)\,\Psi(x_2)\,\Psi(x_1)\,dx_1dx_2\end{gathered}$$

$$\text{Внешнее поле} \quad \sum_{j=1}^{N} U_{\text{ext}}(q_j) \to \int U_{\text{ext}}(q)\Psi^{\dagger}(x)\Psi(x)dx$$

зависимость от времени

$$\begin{gathered}H(t) = e^{i\frac{H}{\hbar}t}He^{-i\frac{H}{\hbar}t} = H, \quad \mathbf{H} = -\tfrac{\hbar^2}{2m}\int \Psi^{\dagger}(t,x)\Delta_q\Psi(t,x)dx + \\ +\tfrac{1}{2}\iint V(q_1-q_2)\,\Psi^{\dagger}(t,x_1)\,\Psi^{\dagger}(t,x_2)\,\Psi(t,x_2)\,\Psi(t,x_1)\,dx_1dx_2 = \\ = -\tfrac{\hbar^2}{2m}\int \Psi^{\dagger}(x)\triangle_q\Psi(x)dx + \tfrac{1}{2}\iint V(q_1-q_2)\,\Psi^{\dagger}(x_1)\,\Psi^{\dagger}(x_2)\,\Psi(x_2)\,\Psi(x_1)\,dx_1dx_2\end{gathered}$$

$$\begin{gathered}\mathfrak{A} = \sum_{j=1,\ldots,N} A_j; \quad \mathbf{A} = \int \Psi^{\dagger}(x)A(x,y)\Psi(y)dydx = \\ = \int \sum_{f,g}\psi_f^*(x)a_f^{\dagger}A(x,y)\psi_g(y)a_gdydx = \sum_{f,g}\langle f|A|g\rangle a_f^{\dagger}a_g\end{gathered}$$

$$\langle f|A|g\rangle \equiv \int \psi_f^*(x)A(x,y)\psi_g(y)dydx$$

$$\mathbf{B} = \tfrac{1}{2}\iint V(q_1-q_2)\,\Psi^\dagger(x_1)\,\Psi^\dagger(x_2)\,\Psi(x_2)\,\Psi(x_1)\,dx_1dx_2 = \\ = \tfrac{1}{2}\sum_{f,g,h,i}\langle fg|V|hi\rangle a_f^\dagger a_g^\dagger a_i a_h$$

$$\langle fg|V|hi\rangle \equiv \iint \psi_f^*(x_1)\,\psi_g^*(x_2)\,V(q_1-q_2)\,\psi_h(x_1)\,\psi_i(x_2)\,dx_1dx_2$$

теперь с операторами конец

Гамильтониан и метод Хартри-Фока

$$H = \sum_{i=1}^{N} T(\mathbf{r}_i) + \tfrac{1}{2}\sum_{i\neq j=1}^{N} V(\mathbf{r}_i,\mathbf{r}_j)$$
$$H = \sum_{k,l}\langle k|T|l\rangle a_k^\dagger a_l + \tfrac{1}{2}\sum_{k,l,m,n}\langle kl|V|mn\rangle a_k^\dagger a_l^\dagger a_n a_m$$

где

$$\langle k|T|l\rangle \equiv \int \phi_k^*(\mathbf{r})T(\mathbf{r})\phi_l(\mathbf{r})d\mathbf{r}$$
$$\langle kl|V|mn\rangle \equiv \int \phi_k^*(\mathbf{r}_1)\,\phi_l^*(\mathbf{r}_2)\,V(\mathbf{r}_1,\mathbf{r}_2)\,\phi_m(\mathbf{r}_1)\,\phi_n(\mathbf{r}_2)\,d\mathbf{r}_1d\mathbf{r}_2$$
$$a_k^\dagger a_l^\dagger + a_l^\dagger a_k^\dagger = 0, \quad a_k a_l + a_l a_k = 0, \quad a_k a_l^\dagger + a_l^\dagger a_k = \delta(k-l)$$
$$|\Phi\rangle = \textstyle\prod_{h=1}^{N} a_h^\dagger|0\rangle, \quad \forall k: a_k|0\rangle = 0; \quad \langle\Phi|H|\Phi\rangle = \min, \quad \delta\langle\Phi|H|\Phi\rangle = 0$$
$$\Phi(\mathbf{r}_1,...,\mathbf{r}_N) = \tfrac{1}{\sqrt{N!}}\begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_1(\mathbf{r}_2) & ... & \phi_1(\mathbf{r}_N) \\ \phi_2(\mathbf{r}_1) & \phi_2(\mathbf{r}_2) & ... & \phi_2(\mathbf{r}_N) \\ ... & ... & ... & ... \\ \phi_N(\mathbf{r}_1) & \phi_N(\mathbf{r}_2) & ... & \phi_N(\mathbf{r}_N) \end{vmatrix}$$

Как варьировать определитель Слэтера

$$\delta\langle\Phi|H|\Phi\rangle = 0 \Longleftrightarrow \langle\delta\Phi|H|\Phi\rangle = 0, \quad \langle\Phi|H|\delta\Phi\rangle = 0$$
$$\phi_h(\mathbf{r}) \to \phi_h(\mathbf{r}) + \eta\phi_p(\mathbf{r}), \quad 1 \leqslant h \leqslant N, p > N$$
$$|\delta\Phi\rangle = \eta a_p^\dagger a_h|\Phi\rangle: \quad \left\langle\Phi\left|Ha_p^\dagger a_h\right|\Phi\right\rangle = 0, \quad \left\langle\Phi\left|a_h^\dagger a_p H\right|\Phi\right\rangle = 0$$

Средние по состоянию Х-Ф

$$\langle k|T|l\rangle: \quad \left\langle\Phi\left|a_h^\dagger a_p a_k^\dagger a_l\right|\Phi\right\rangle = \left\langle\Phi\left|a_h^\dagger\left(\delta(k-p) - a_k^\dagger a_p\right)a_l\right|\Phi\right\rangle \\ = \delta(k-p)\left\langle\Phi\left|a_h^\dagger a_l\right|\Phi\right\rangle - \left\langle\Phi\left|a_h^\dagger a_k^\dagger a_p a_l\right|\Phi\right\rangle = \delta(k-p)\delta(l-h)$$

$$\langle kl|V|mn\rangle: \quad \left\langle\Phi\left|a_h^\dagger a_p a_k^\dagger a_l^\dagger a_n a_m\right|\Phi\right\rangle = \left\langle\Phi\left|a_h^\dagger\left(\delta(k-p) - a_k^\dagger a_p\right)a_l^\dagger a_n a_m\right|\Phi\right\rangle = \\ = -\delta(k-p)\delta(n-h)\left\langle\Phi\left|a_l^\dagger a_m\right|\Phi\right\rangle + \delta(l-p)\left\langle\Phi\left|a_k^\dagger a_h^\dagger a_n a_m\right|\Phi\right\rangle + \\ +\delta(k-p)\left\langle\Phi\left|a_l^\dagger a_n a_h^\dagger a_m\right|\Phi\right\rangle =$$

уравнение Фадеева для трех тел

уравнение Фадеева-Якубовского для четырех тел

Типичные системы из многих частиц (???)

Открытые системы из многих частиц (???)

(хз, но такие есть тоже, см. кв. теор инф)

25.4 Special Applications of Path Integral Methods

25.4.1 Path Integral Approach for Gravitational Lensing

(discuss how to use it here. write some comments in the theory of path integral. so, in general this is our deeper understanding of path integral, that is why I'll be working on the section about path integral!)

25.4.2 Path Integral Approach for Gravitational Lensing: Background and Features

(there are many things which are assumed here and many connections with other topics, so I'll create a short summary of them)

25.5 Introduction to Other Questions

(big books are written about all things in each subsubsection here.)

25.5.1 Quantum Phenomena in Astronomy

(да, там используется квантмех, тут подготовка для этих явлений, а подробно буду писать в записи по астрономии.)

Обзор применений в астрономии

(пока не очень шарю, потом мб посмотрю.)

Про источники энергии звезд

Теория

В 1929 г. Р. Аткинсон и Ф. Хоутерманс (1903 – 1966) высказали гипотезу о том, что внутри Солнца и других звезд существуют условия для протекания реакций ядерного синтеза, и их излучение создается за счет термоядерных реакций.

В настоящее время принято считать, что Солнце и звезды образовались (и образуются) в результате постепенной гравитационной конденсации межзвездного газа, состоящего в основном из водорода.

В первоначальной фазе сжатия, которая для звезды с массой, близкой к массе Солнца, длится около 10^7 лет, температура звезды повышается только за счет гравитационной энергиИ.

Когда температура внутренних областей достигает 10^7K, они превращаются в горячую плазму и начинаются ядерные реакции водородного цикла, при которых четыре ядра водорода в конечном счете превращаются в ядро ^{4}He с выделением около 26,2 МэВ энергии.

Эти реакции происходят через ряд последовательных ступеней:

$$
\begin{aligned}
{}^1\mathrm{H} + {}^1\mathrm{H} &\to {}^2\mathrm{H} + e^+ + \nu \\
{}^2\mathrm{H} + {}^1\mathrm{H} &\to {}^3\mathrm{He} + \gamma \\
{}^3\mathrm{He} + {}^3\mathrm{He} &\to {}^4\mathrm{He} + 2{}^1\mathrm{H} \\
{}^3\mathrm{He} + {}^4\mathrm{He} &\to {}^7\mathrm{Be} + \gamma \\
{}^7\mathrm{Be} + {}^1\mathrm{H} &\to {}^8\ \mathrm{B} \to {}^8\mathrm{Be} + e^+ + \nu \\
{}^8\mathrm{Be} &\to 2{}^4\mathrm{He} \\
{}^7\mathrm{Be} + e^- &\to {}^7\mathrm{Li} + \nu \\
{}^7\mathrm{Li} + {}^1\mathrm{H} &\to 2{}^4\mathrm{He}
\end{aligned}
$$

состоит из водорода и гелия.

Это дает основание предположить, что источником энергии Солнца действительно служит превращение водорода в гелий. Гидродинамическое и тепловое равновесие в звезде обеспечивается равенством сил тяготения и давления, действующих на каждый элемент ее массы.

Выделение ядерной энергии компенсирует потери энергии на излучение.

Длительность данной стадии зависит от массы звезды и от запасов водорода. Другой возможный процесс превращения водорода в гелий был предложен Г. Бете (19062005).

Он называется углеродным циклом.

Протекание углеродного цикла возможно в звездах, которые уже содержат достаточное количество ядер атомов углерода и кислорода, служащих катализаторами.

Он состоит из последовательности реакций:

$$
\begin{aligned}
12\mathrm{C} + {}^1\mathrm{H} &\to {}^{13}\mathrm{H} + \gamma \\
{}^{13}\ \mathrm{N} &\to {}^{13}\mathrm{C} + e^+ + \nu\,(1,2\mathrm{M}_\ni\mathrm{B})\,, \\
{}^1\mathrm{H} + {}^{13}\mathrm{C} &\to {}^{14}\ \mathrm{N} + \gamma \\
{}^1\mathrm{H} + {}^{14}\ \mathrm{N} &\to {}^{15}\mathrm{O} + \gamma \\
{}^{15}\mathrm{O} &\to {}^{15}\ \mathrm{N} + e^+ + \nu\,(1,7\mathrm{M}_\ni\mathrm{B})\,, \\
{}^1\mathrm{H} + {}^{15}\ \mathrm{N} &\to {}^{12}\mathrm{C} + {}^4\mathrm{He}
\end{aligned}
$$

в результате которых четыре ядра водорода превращаются в ядро ^{4}He с выделением около $25\mathrm{M}_\ni\mathrm{B}$, как и при водородном цикле.

Поведение ядра углерода в данном случае очень похоже на поведение катализаторов при химических реакциях, сохраняющихся после завершения цикла.

На Солнце, по-видимому, главную роль играет водородный цикл.

Каждую секунду в нем около $8 \cdot 10^8$ т водорода превращается в гелий.

Если этот процесс будет продолжаться с той же интенсивностью, то запасов водорода хватит еще на 10^{10} лет.

Интересно, что около 5% энергии Солнца и звезд, в которых энергия выделяется в результате водородного цикла, излучается в виде нейтрино.

История открытия

(скину сюда все разное)

модели космоса

тут покажем, как квантовая физика описывает многие астрономические явления.
(мб квантовую космологию посмотрю)

26 Advanced Exotic Mathematical Methods of Quantum Mechanics

Here, I'll put purely mathematical theories which I have no idea how to use or which have not been used much by others.

(I'll move some theory from theoretical sections here. From Takhtajayan and others, there are a lot of such methods)

26.1 Supersymmetry

26.1.1 Why Does One Need Supersymmetry and What Does It Give?

(a very important question, I'll write it here)

26.1.2 Supermanifolds

The coordinate vector space $V = \mathbb{R}^n$ has a natural structure of a smooth manifold, which to every open subset $U \subseteq \mathbb{R}^n$ assigns a commutative $\mathbb{R}$ algebra $C^\infty(U)$ of all smooth functions on U. The assignment

$$U \mapsto C^\infty(U)$$

for all open $U \subseteq \mathbb{R}^n$ defines a sheaf of commutative $\mathbb{R}$-algebras (commutative rings) on a topological space $\mathbb{R}^n$, and turns it into a ringed space. Every smooth n-dimensional manifold M is a ringed space - a topological space with a sheaf of commutative rings, which is locally isomorphic to the ringed space $\mathbb{R}^n$. It is easy to see that this definition is equivalent to the standard one, defined by gluing coordinate charts. The notion of a supermanifold generalizes this idea by using local models associated with graded vector spaces.

Namely, let $W = \mathbb{R}^{p|q}$ be the coordinate graded vector space of dimension $p|q$ over $\mathbb{R}$. The following definition formalizes the intuitive idea that odd coordinates on W are anticommuting.

Definition. A supermanifold $\mathbb{R}^{p|q}$ is a topological space $\mathbb{R}^p$ with a sheaf of commutative $\mathbb{R}$-superalgebras (supercommutative rings) over $\mathbb{R}$, called the structure sheaf, defined by the assignment

$$U \mapsto C^\infty(U)\left[\theta^1, ..., \theta^q\right]$$

for all open $U \subseteq \mathbb{R}^p$, where $C^\infty(U)\left[\theta^1, ..., \theta^q\right]$ is a Grassmann algebra with generators $\theta^1, ..., \theta^q$ over the commutative ring $C^\infty(U)$.

Remark. Elements of $C^\infty(U)\left[\theta^1, ..., \theta^q\right]$ have the form

$$f = \sum_I f_I \theta^I, \quad \theta^I = \theta^{i_1} ... \theta^{i_k} \quad \text{and} \quad f_I \in C^\infty(U)$$

for $I = \{i_1, ..., i_k\} \subset \{1, ..., q\}$, and are called functions on a supermanifold $\mathbb{R}^{p|q}$ over U. Thus $\mathbb{R}^{p|q}$ is a coordinate space with even coordinates $\boldsymbol{x} = (x^1, ..., x^p)$ and odd coordinates $\boldsymbol{\theta} = (\theta^1, ..., \theta^q)$, and we will write $f \in C^\infty(U)\left[\theta^1, ..., \theta^q\right]$ as $f(\boldsymbol{x}, \boldsymbol{\theta})$.

Definition. A supermanifold of dimension $p|q$ is a pair $(X, \mathcal{O}_X)$ - a topological space X with a sheaf $\mathcal{O}_X$ of supercommutative rings over $\mathbb{R}$, called the structure sheaf, which is locally isomorphic to $\mathbb{R}^{p|q}$.

Supermanifolds form a category: a morphism between supermanifolds $(X, \mathcal{O}_X)$ and $(Y, \mathcal{O}_Y)$ is a continuous map $\varphi : X \to Y$, together with a sheaf map $\varphi^* : \mathcal{O}_Y \to \mathcal{O}_X$ over φ, a collection of homomorphisms of supercommutative rings over $\mathbb{R}$,

$$\varphi_V^* : \mathcal{O}_Y(V) \to \mathcal{O}_X\left(\varphi^{-1}(V)\right), \quad V \subseteq Y \quad \text{open}$$

which commute with restriction maps of the sheaves.

To every vector bundle E of rank q over an ordinary p-dimensional manifold M there is an associated supermanifold ΠE of dimension $p|q$, defined by reversing parity in the fibers of E. Namely, for every open $U \subseteq M$ let $C^\infty(U, E)$ be the space of all smooth sections of E over U. It is a free $C^\infty(U)$ module generated by q sections $\theta^1, ..., \theta^q$. Consider them as generators of the Grassmann algebra (this explains using Greek letters), and define the structure sheaf of ΠE by the assignment $U \mapsto C^\infty(U)\left[\theta^1, ..., \theta^q\right]$. It can be shown that every supermanifold is isomorphic (non-canonically) to ΠE for some vector bundle E over M.

Remark. Supermanifolds have many more morphisms than vector bundles, since one is allowed to mix even and odd variables. Thus for the supermanifold $\mathbb{R}^{1|2}$ with even coordinate x and odd coordinates θ_1, θ_2 the mapping

$$\varphi(x) = x + \theta^1\theta^2, \quad \varphi\left(\theta^i\right) = \theta^i, \quad i = 1, 2$$

is an isomorphism of $\mathbb{R}^{1/2}$, but it is not induced by an isomorphism of a trivial rank 2 vector bundle over $\mathbb{R}$.

Using these definitions, one can develop differential geometry of supermanifolds and the corresponding theory of integration, which is quite similar to that for ordinary manifolds (see Section 7 for the references). Here we will only consider the simplest example of supermanifolds ΠTM, where M is an ordinary manifold. It is quite remarkable that the basic notions of differential geometry on a manifold M can be formulated in terms of the supermanifold $\Pi\mathrm{T}\, M$.

Namely, let $\mathcal{A}^\bullet(M)$ be a commutative superalgebra of smooth differential forms on the n-dimensional manifold M, and let $C^\infty(\Pi TM)$ be a commutative superalgebra of global sections of the structure sheaf of ΠTM - the superalgebra of functions on a supermanifold ΠTM. The isomorphism

$$\mathcal{A}^\bullet(M) \simeq C^\infty(\Pi TM)$$

allows us to interpret differential forms on M as functions on ΠTM. Indeed, to every $\omega_p \in \mathcal{A}^p(M)$, given in local coordinates on $U \subset M$ by

$$\omega_p = \sum_{1 \le i_1 < \cdots < i_p \le n} a_{i_1 \ldots i_p}(\boldsymbol{x}) dx^{i_1} \wedge \cdots \wedge dx^{i_p}$$

we assign

$$\omega_p(\boldsymbol{x}, \boldsymbol{\theta}) = \sum_{1 \le i_1 < \cdots < i_p \le n} a_{i_1 \ldots i_p}(\boldsymbol{x}) \theta^{i_1} \ldots \theta^{i_p} \in C^\infty(U)\left[\theta^1, ..., \theta^n\right].$$

It trivially follows from the definition of differential form and of ΠTM that under a change of coordinates $a_{i_1 \ldots i_p}(\boldsymbol{x})$ transform like coefficients of differential forms, and $\theta^1, ..., \theta^n$ transform like components of tangent vectors, so that $\omega_p(\boldsymbol{x}, \boldsymbol{\theta})$ is a well-defined function on the supermanifold ΠTM. Correspondingly, the de Rham differential d gives rise to an odd vector field δ on ΠTM,

$$\delta = \sum_{k=1}^{n} \theta^k \frac{\partial}{\partial x^k},$$

with the property that $\delta^2 = 0$. Finally, the supermanifold ΠTM carries a canonical volume form $d\boldsymbol{x}d\boldsymbol{\theta} = dx^1...dx^n d\theta^1...d\theta^n$, which is well defined due to the opposite change of variables formulas for the ordinary and Berezin's integrals (see Section 2.3 of Chapter 7). The integration of a top differential form over M reduces to the integration of a corresponding function over ΠTM with respect to the canonical volume form,

$$\int_M \omega_n = \int_{\Pi TM} \omega_n(\boldsymbol{x}, \boldsymbol{\theta}) d\boldsymbol{x} d\boldsymbol{\theta}$$

Remark. Sometimes in the mathematics literature, in order to emphasize the opposite change of variables formulas for the ordinary and Berezin's integrals, the volume form on the supermanifold ΠTM is denoted by $d\boldsymbol{x}d\boldsymbol{\theta}^{-1}$.

Problem 1.1. Prove all statements in this section.

26.1.3 Equivariant Cohomology and Localization

2.1. Finite-dimensional case.

Let M be a compact orientable n-dimensional manifold with the circle action - an action of abelian group $U(1) = S^1$ - and let $V \in \mathrm{Vect}(M)$ be the vector field corresponding to this action,

$$V(f)(x) = \left.\frac{d}{dt}\right|_{t=0} f\left(e^{it} \cdot x\right), \quad x \in M.$$

Consider the linear operator

$$D = d - i_V : \mathcal{A}^\bullet(M) \to \mathcal{A}^\bullet(M),$$

where i_V is the inner product operator with V. Using the identification $\mathcal{A}^\bullet(M) \simeq C^\infty(\Pi TM)$, in local coordinates $\boldsymbol{x} = (x^1, ..., x^n)$ on $U \subset M$ we can represent D by

$$D = \sum_{\mu=1}^n \left(\theta^\mu \frac{\partial}{\partial x^\mu} - v^\mu \frac{\partial}{\partial \theta^\mu}\right), \quad \text{where} \quad V = \sum_{\mu=1}^n v^\mu \frac{\partial}{\partial x^\mu}. \tag{2.1}$$

It follows from the Cartan formula (see Chapter 1), or directly from (2.1), that

$$D^2 = -\mathcal{L}_V,$$

where $\mathcal{L}_V$ is a Lie derivative. Thus D is a differential on the subcomplex $\mathcal{A}^\bullet(M)^{S^1}$ of S^1-invariant differential forms on M. The cohomology of this complex is an equivariant cohomology in the Cartan formulation. Since d and i_V have, respectively, degrees 1 and -1 , equivariantly closed forms on M necessarily have several components. Namely, the equation $D\alpha = 0$ for $\alpha = \sum_{p=0}^n \alpha_p \in \mathcal{A}^\bullet(M)$ is equivalent to the following system of equations:

$$d\alpha_p = i_V \alpha_{p+2}, \quad p = 0, ..., n-2, \quad \text{and} \quad d\alpha_{n-1} = 0.$$

Let M_V be a zero locus of the vector field V - the set of fixed points of the circle action. We have the following fundamental property of equivariantly closed differential forms.

Lemma 2.1. An equivariantly closed differential form an a compact manifold M is equivariantly exact on $M \backslash M_V$.

Proof. Let $\alpha \in \mathcal{A}^\bullet(M)$ be such that $D\alpha = 0$. We want to find a differential form λ on $M \backslash M_V$ such that $\alpha = D\lambda$ on $M \backslash M_V$. Suppose there is a form ξ on $M \backslash M_V$, with components of odd degrees, satisfying $D\xi = 1$. Setting $\lambda = \xi \wedge \alpha$ we get

$$D\lambda = D\xi \wedge \alpha - \xi \wedge D\alpha = \alpha$$

To construct such a form ξ, choose an S^1-invariant Riemannian metric g on M, and denote by $\beta \in \mathcal{A}^1(M)$ the 1-form on M dual to the vector field V with respect to the Riemannian metric, $\beta = \langle V, \cdot \rangle$. Since the metric g is S^1-invariant, $\mathcal{L}_V g = 0$ and, therefore, $\mathcal{L}_V \beta = 0$. We have

$$D\beta = K + \Omega, \quad \text{where} \quad K = -\|V\|^2 \quad \text{and} \quad \Omega = d\beta.$$

Since $K \in \mathcal{A}^0(M)$ does not vanish on $M \backslash M_V$,

$$\xi = \beta(D\beta)^{-1} = \frac{\beta}{K}\left(1 + K^{-1}\Omega\right)^{-1} = \frac{\beta}{K}\sum_{i=0}^{l}(-1)^i\frac{\Omega^i}{K^i}, \quad l = \left[\frac{n}{2}\right],$$

is a well-defined form on $M \backslash M_V$ satisfying $D\xi = 1$.

Corollary 2.1. The top component of an equivariantly closed form on M is exact on $M \backslash M_V$.

Remark. In local coordinates $\boldsymbol{x} = (x^1, ..., x^n)$ on M the Riemannian metric g has the form [1] $ds^2 = g_{\mu\nu}dx^\mu dx^\nu$, and equation $\mathcal{L}_V g = 0$ - the condition that V is a Killing vector field with respect to the metric g - can be written as

$$g_{\mu\lambda}\nabla_\nu v^\lambda + g_{\nu\lambda}\nabla_\mu v^\lambda = 0. \tag{2.2}$$

Here ∇_μ is a covariant derivative with respect to the vector field $\frac{\partial}{\partial x^\mu}$. For the 1 -form $\beta = g_{\mu\nu}v^\nu dx^\mu$ we also have

$$D\beta = -g_{\mu\nu}v^\mu v^\nu + \omega_{\mu\nu}dx^\mu \wedge dx^\nu, \quad \text{where} \quad \omega_{\mu\nu} = g_{\nu\lambda}\nabla_\mu v^\lambda. \tag{2.3}$$

By (2.2), the $n \times n$ matrix $\omega(\boldsymbol{x}) = \{\omega_{\mu\nu}(\boldsymbol{x})\}_{\mu,\nu=1}^n$ is skew-symmetric. For even $n = 2l$, orientation on M allows us to define $\mathrm{Pf}(\omega(x))$ as the product $\lambda_1 ... \lambda_l$ of above-diagonal elements in the canonical form [2] of a skewsymmetric matrix $\omega(\boldsymbol{x})$ (see Section 2.3 of Chapter 7). Correspondingly, $\mathrm{Pf}(\omega)(\boldsymbol{x})(\det g(\boldsymbol{x}))^{-\frac{1}{2}}$ does not depend on a choice of local coordinates, and defines a function on M. For every $x \in M$ there is also a linear mapping $L_x : T_xM \to T_xM$, defined by $L_x W = (\nabla_W V)(x)$, where ∇_W is a covariant derivative with respect to $W \in T_xM$. Since $\det L_x \det g(x) = \mathrm{Pf}(\omega(x))^2$, we define

$$\sqrt{\det L_x} = \frac{\mathrm{Pf}(\omega(x))}{\sqrt{\det g(x)}}. \tag{2.4}$$

For $x \in M_V$ the mapping L_x does not depend on the choice of an S^1-invariant metric g, and is given by the matrix $\left\{\frac{\partial v^\mu}{\partial x^\nu}(\boldsymbol{x})\right\}_{\mu,\nu=1}^n$.

According to Lemma 2.1, the integral $\int_M \alpha$ of an equivariantly closed differential form α localizes on the zero locus M_V. A quantitative result is given by the following statement.

Proposition 2.1. Suppose that $D\alpha = 0$ on M. Then for every S^1-invariant $\beta \in \mathcal{A}^1(M)$ the integral $\int_M \alpha e^{tD\beta}$ does not depend on t.

Proof. Denote this integral by $Z(t)$. We have

$$\frac{dZ}{dt} = \int_M \alpha D\beta e^{tD\beta} = \int_M D\left(\beta\alpha e^{tD\beta}\right) + \int_M \beta D\left(\alpha e^{tD\beta}\right) = 0$$

where the first integral is zero by Stokes' theorem, and the second integral is zero by the conditions $D\alpha = 0$ and $D^2\beta = 0$.

[01] We are assuming the summation over repeated indices.

[2] Obtained by using orthogonal transformation with determinant 1 .

This result is usually used to evaluate $Z(0) = \int_M \alpha$ by computing the asymptotics of $Z(t)$ as $t \to \infty$. For a suitably chosen 1-form β the leading contribution is given by the integral over a tubular neighborhood of the zero locus of the component $K = (D\beta)_0 \in \mathcal{A}^0(M)$, which can be computed in the closed form as $t \to \infty$. The simplest case of a localization phenomenon is when the circle action on M has only isolated fixed points, i.e., when M_V is a finite set and L_x is non-degenerate for $x \in M_V$. In particular, in this case n is even.

Theorem 2.2 (Berline-Vergne localization theorem). Let M be a compact oriented $2l$-dimensional manifold with a circle action which has only isolated fixed points. Then for every equivariantly closed form $\alpha \in \mathcal{A}^\bullet(M)$,

$$\int_M \alpha = (2\pi)^l \sum_{x \in M_V} \frac{\alpha_0(x)}{\sqrt{\det L_x}}.$$

Proof. Let β be the 1-form introduced in the proof of Lemma 2.1, so that in local coordinates $\Omega = d\beta = \omega_{\mu\nu} dx^\mu \wedge dx^\nu$. Using Proposition 2.1 and the identification $\mathcal{A}^\bullet(M) \simeq C^\infty(\Pi TM)$, we get

$$\int_M \alpha = \lim_{t\to\infty} \int_{\Pi TM} \alpha(\boldsymbol{x}, \boldsymbol{\theta}) e^{-t g_{\mu\nu}(\boldsymbol{x}) v^\mu(\boldsymbol{x}) v^\nu(\boldsymbol{x}) + t\omega_{\mu\nu}(\boldsymbol{x})\theta^\mu\theta^\nu} d\boldsymbol{x} d\boldsymbol{\theta}$$

We have in the distributional sense,

$$\lim_{t\to\infty} \left(\frac{t}{\pi}\right)^l \sqrt{\det g(\boldsymbol{x})} e^{-t g_{\mu\nu}(\boldsymbol{x}) v^\mu(\boldsymbol{x}) v^\nu(\boldsymbol{x})} = \delta(V(\boldsymbol{x})) \tag{2.5}$$

- the main formula of the method of steepest descent (cf. the method of stationary phase in Section 2.3 of Chapter 2) - and

$$\lim_{t\to\infty} (2t)^{-l} \frac{1}{\mathrm{Pf}(\omega(\boldsymbol{x}))} e^{t\omega_{\mu\nu}(\boldsymbol{x})\theta^\mu\theta^\nu} = \delta(\boldsymbol{\theta}) \tag{2.6}$$

- the main formula of Gaussian integration over Grassmann variables (see Proposition 2.3 in Section 2.3 of Chapter 7). Since $\alpha_0(\boldsymbol{x}) = \alpha(\boldsymbol{x}, 0)$, we obtain the result by using formulas (2.5)-(2.6), (2.4), and

$$\delta(V(\boldsymbol{x})) = \sum_{x_i \in M_V} \frac{1}{|\det L_{x_i}|} \delta(\boldsymbol{x} - \boldsymbol{x}_i).$$

Problem 2.1. Prove formulas (2.2)-(2.4).

Problem 2.2. Prove formulas (2.5)-(2.6) and complete the proof of Theorem 2.2.

2.2. Infinite-dimensional case. An important class of infinite-dimensional manifolds is given by the loop spaces. Let M be a compact orientable n-dimensional manifold and let

$$\mathcal{L}(M) = C^\infty\left(S^1, M\right),$$

where $S^1 = \mathbb{R}/\mathbb{Z}$, be its free loop space. The loop space $\mathcal{L}(M)$ is an infinitedimensional Frchet manifold, and the tangent space $T_\gamma\mathcal{L}(M)$ to $\mathcal{L}(M)$ at a point $\gamma \in \mathcal{L}(M)$ is

$$T_\gamma\mathcal{L}(M) = \Gamma\left(S^1, \gamma^*(TM)\right)$$

- the vector space of smooth vector fields $V = \left\{v(t) \in T_{\gamma(t)}M, 0 \le t \le 1\right\}$ along the loop γ in M.

The loop space $\mathcal{L}(M)$ has a canonical circle action given by the action of S^1 on itself by rotations. The vector field corresponding to this action is $\dot\gamma$ - the velocity vector field $\dot\gamma(t)$ along the loop γ in M. The fixed points of the action are constant loops, so that $\mathcal{L}(M)_{\dot\gamma} = M$.

The vector field $\dot\gamma$ on $\mathcal{L}(M)$ - a generator of the circle action on $\mathcal{L}(M)$ is analogous to the vector field V on M, considered in the previous section. As in the finite-dimensional case, denote by $D = d - i_{\dot\gamma}$ the equivariant differential on the complex $\mathcal{A}^\bullet(\mathcal{L}(M))^{S^1}$ of equivariant differential forms on $\mathcal{L}M$. Using the identification $\mathcal{A}^\bullet(\mathcal{L}(M)) \simeq C^\infty(\Pi T\mathcal{L}(M))$, we have the following infinite-dimensional analog of representation (2.1):

$$DF = \int_0^1 \left(\theta^\mu(t) \frac{\delta F}{\delta x^\mu(t)} - \dot x^\mu(t) \frac{\delta F}{\delta \theta^\mu(t)} \right) dt, \quad F \in C^\infty(\Pi T\mathcal{L}(M)). \tag{2.7}$$

Here we are using functional derivatives (as in calculus of variations), local coordinates $\boldsymbol{x} = (x^1, ..., x^n)$ on M, and associated standard coordinates in $T_{\gamma(t)}M$ and $\Pi T_{\gamma(t)}M$, so that $\dot\gamma(t) = (\dot x^1(t), ..., \dot x^n(t)) \in T_{\gamma(t)}M$ and $\boldsymbol{\theta}(t) = (\theta^1(t), ..., \theta^n(t)) \in \Pi T_{\gamma(t)}M$. As in the finite-dimensional case,

$$D^2 = -\int_0^1 \left(\dot x^\mu(t) \frac{\delta}{\delta x^\mu(t)} + \dot\theta^\mu(t) \frac{\delta}{\delta \theta^\mu(t)} \right) dt = -\mathcal{L}_{\dot\gamma}. \tag{2.8}$$

To define the infinite-dimensional analog of a 1 -form β, we choose a Riemannian metric $g_{\mu\nu}dx^\mu dx^\nu$ on M and consider an S^1-invariant Riemannian metric on $\mathcal{L}(M)$, obtained by the integration of g along a loop [3],

$$\langle V_1, V_2 \rangle_\gamma = \int_0^1 \langle v_1(t), v_2(t) \rangle \, dt, \quad V_1, V_2 \in T_\gamma \mathcal{L}(M).$$

The 1 -form β on $\mathcal{L}(M)$ is dual to the vector field $\dot\gamma$ with respect to the Riemannian metric on $\mathcal{L}(M)$, and is given by the following function on $\Pi T\mathcal{L}(M)$:

$$\beta(\gamma, \theta) = \int_0^1 \langle \dot\gamma(t), \boldsymbol{\theta}(t) \rangle dt = \int_0^1 g_{\mu\nu}(\gamma(t)) \dot x^\mu(t) \theta^\nu(t) dt. \tag{2.9}$$

Lemma 2.2. The 1 -form β on $\mathcal{L}(M)$ is S^1 invariant, and the function $D\beta = -2S$ on $\Pi T\mathcal{L}(M)$ is given by

$$S(\gamma, \theta) = \frac{1}{2} \int_0^1 \left(\|\dot\gamma(t)\|^2 + \left\langle \boldsymbol{\theta}(t), \nabla_{\dot\gamma(t)} \boldsymbol{\theta}(t) \right\rangle \right) dt \tag{2.10}$$

where $\nabla_{\dot\gamma}$ is a covariant derivative along γ. The first term in $-2S$ is an analog of the function K in the finite-dimensional case, and the second term is an analog of the 2 -form Ω.

Proof. The 1 -form β is S^1-invariant by definition. We have

$$D\beta = d\beta - i_{\dot\gamma}\beta,$$

where the second term, a function $-i_{\dot\gamma}\beta$ on $\Pi T\mathcal{L}(M)$, clearly gives the first term in (2.10). Now using that in the distributional sense

$$\frac{\delta}{\delta x^\rho(s)} x^\mu(t) = \delta^{\rho\mu} \delta(t - s)$$

and

[03] Here and in what follows $\langle v_1(t), v_2(t) \rangle$ always stands for the inner product in $T_{\gamma(t)}M$ given by the Riemannian metric g.

$$\frac{\delta}{\delta x^\rho(s)}\dot{x}^\mu(t) = \delta^{\rho\mu}\frac{d}{dt}\delta(t-s) = -\delta^{\rho\mu}\frac{d}{ds}\delta(t-s),$$

we compute the term $d\beta$ as follows:

$$\begin{aligned} d\beta(\gamma,\theta) &= \int_0^1\int_0^1 \theta^\rho(s)\frac{\delta}{\delta x^\rho(s)}\left(g_{\mu\nu}(\boldsymbol{x}(t))\dot{x}^\mu(t)\right)\theta^\nu(t)dsdt \\ &= \int_0^1\int_0^1 \theta^\rho(s)\left(\frac{\partial g_{\mu\nu}}{\partial x^\rho}\dot{x}^\mu(t)\delta(t-s) - \delta^{\rho\mu}g_{\mu\nu}\frac{d}{ds}\delta(t-s)\right)\theta^\nu(t)dsdt \\ &= \int_0^1 \left(g_{\mu\nu}(\boldsymbol{x}(t))\dot{\theta}^\mu(t)\theta^\nu(t) + \frac{\partial g_{\mu\nu}}{\partial x^\rho}(\boldsymbol{x}(t))\dot{x}^\mu(t)\theta^\rho(t)\theta^\nu(t)\right)dt. \end{aligned}$$

It follows from the definition of Christoffel's symbols (see Example 1.7 in Section 1.3 of Chapter 1) and anticommutativity of θ^μ that

$$\frac{\partial g_{\mu\nu}}{\partial x^\rho}\dot{x}^\mu\theta^\rho\theta^\nu = g_{\mu\nu}\Gamma^\nu_{\lambda\sigma}\dot{x}^\lambda\theta^\mu\theta^\sigma, \tag{2.11}$$

and we obtain

$$\begin{aligned} d\beta(\gamma,\theta) &= \int_0^1 g_{\mu\nu}(\boldsymbol{x}(t))\left(\dot{\theta}^\mu(t) + \Gamma^\mu_{\sigma\lambda}(\boldsymbol{x}(t))\dot{x}^\sigma(t)\theta^\lambda(t)\right)\theta^\nu(t)dt \\ &= \int_0^1 \left\langle \nabla_{\dot{\gamma}(t)}\boldsymbol{\theta}(t), \boldsymbol{\theta}(t)\right\rangle dt. \end{aligned}$$

As in Chapter 6, one can develop the integration theory on $\mathcal{L}(M)$ with respect to the Wiener measure associated with a Riemannian metric on M by using the corresponding heat kernel [4]. One can also integrate differential forms over $\mathcal{L}(M)$, provided that $\mathcal{L}(M)$ is orientable. As in the finitedimensional case, the latter is defined by the condition that the structure group of an $\mathcal{L}(\mathrm{SO}(n))$-bundle $\mathcal{L}(FM) \to \mathcal{L}(M)$, where $FM \to M$ is the frame bundle, reduces to the connected component of the identity. It follows from the transgression homomorphism

$$H^2(M,\mathbb{Z}_2) \to H^1(\mathcal{L}(M),\mathbb{Z}_2)$$

that the image of the second Stiefel-Whitney class of M is the obstruction to orientability of $\mathcal{L}(M)$. In particular, if M is a spin manifold, then $\mathcal{L}(M)$ is orientable, and if M is simply connected, then this is also a necessary condition.

In what follows we will not attempt to develop the integration theory on $\mathcal{L}(M)$, and will formulate and "prove" the infinite-dimensional version of the general Berline-Vergne localization theorem at a heuristic level only. The key observation, by Lemma 2.2, is that the differential form e^{-S} on $\mathcal{L}(M)$ is equivariantly closed, therefore the functional integral $\int_{\mathcal{L}(M)} e^{-S}$ localizes reduces to the finite-dimensional integral over $\mathcal{L}(M)_{\dot{\gamma}} = M$, the zero locus of the vector field $\dot{\gamma}$.

To give the quantitative formulation of this result, recall the notion of the $\hat{A}$-genus. Namely, the $\hat{A}$-genus of a Riemannian manifold (M,g) is a differential form $\hat{A}(M)$, defined as follows. Let $R \in \mathcal{A}^2(M,\mathfrak{so}(TM))$ be the Riemannian curvature of M, and let e_μ be a local orthonormal frame of TM. Put

$$\mathrm{R}_{\mu\nu} = (Re_\mu, e_\nu) \in \mathcal{A}^2(M)$$

and let

$$j(\mathrm{R}) = \det\left(\frac{\sinh \mathrm{R}/2}{\mathrm{R}/2}\right)$$

be an even degree differential form on M. It does not depend on the choice of a local orthonormal frame of TM, and the $\hat{A}$-genus of the manifold M is defined by [5]

$$\hat{A}(M) = j(\mathrm{R})^{-\frac{1}{2}} = \det\left(\frac{\mathrm{R}/2}{\sinh \mathrm{R}/2}\right)^{\frac{1}{2}} \in \mathcal{A}^{\bullet}(M)$$

It is a closed differential form, whose cohomology class does not depend on the choice of a Riemannian metric on M.

Remark. In local coordinates on M,

$$\mathrm{R}_{\mu\nu} = \frac{1}{2} R_{\mu\nu\rho\sigma} dx^{\rho} \wedge dx^{\sigma},$$

where $R_{\mu\nu\rho\sigma}$ is the Riemann curvature tensor.

Theorem 2.3. Let M be a compact orientable manifold such that the free loop space $\mathcal{L}(M)$ is orientable. Then

$$\int_{\mathcal{L}(M)} e^{-S} = (2\pi i)^{-\frac{n}{2}} \int_{M} \hat{A}(M).$$

Proof. The proof is at a heuristic level of rigor. The integral

$$\int_{\mathcal{L}(M)} e^{-S} = \int_{\Pi T\mathcal{L}(M)} e^{-S(\gamma,\theta)} \mathscr{D}\boldsymbol{x} \mathscr{D}\boldsymbol{\theta}$$

localizes at the zero locus $\mathcal{L}(M)_{\dot{\gamma}} = M$, so it is sufficient to integrate over a small tubular neighborhood of ΠTM in $\Pi T\mathcal{L}(M)$. For this aim, consider Riemann normal coordinates of the normal bundle $\mathcal{N}(\Pi TM)$ to ΠTM at a point $(x_0, \theta_0) \in \Pi T_{x_0} M$, given by $\boldsymbol{y}(t) = (y^1(t), ..., y^n(t)) \in T_{x_0} M$ and $\boldsymbol{\eta}(t) = (\eta^1(t), ..., \eta^n(t)) \in \Pi T_{x_0} M$, satisfying

$$\int_0^1 y^{\mu}(t) dt = 0 \quad \text{and} \quad \int_0^1 \eta^{\mu}(t) dt = 0, \quad \mu = 1, ..., n$$

Coordinates $(\varepsilon \boldsymbol{y}(t), \varepsilon \boldsymbol{\eta}(t))$, where real ε is sufficiently small, correspond to a point $\left(\exp_{x_0}(\varepsilon \boldsymbol{y}(t)), P_{(\varepsilon,t)}\left(\theta_0 + \boldsymbol{\eta}(t)\right)\right)$, in the normal bundle $\mathcal{N}(\Pi TM)$, where $\exp_{x_0}$ is the exponential map, and $P_{(\varepsilon,t)}$ is a parallel transport in ΠTM from x_0 along the path $\exp_{x_0}(sy(t))$ as s changes from 0 to ε.

Since we are integrating over an arbitrarily small tubular neighborhood of ΠTM in $\Pi T\mathcal{L}(M)$, it is sufficient to expand $S(\gamma, \theta)$ up to terms of second order in local coordinates $(\boldsymbol{y}(t), \boldsymbol{\eta}(t))$. Since in Riemann normal coordinates around x_0 on M

$$g_{\mu\nu}(\boldsymbol{x}) = \delta_{\mu\nu} + O\left(\|\boldsymbol{x}\|^2\right) \quad \text{and} \quad R_{\mu\nu\rho\sigma}(x_0) = \frac{\partial \Gamma^{\rho}_{\nu\sigma}}{\partial x^{\mu}} - \frac{\partial \Gamma^{\rho}_{\mu\sigma}}{\partial x^{\nu}}$$

we readily obtain that at $(x_0, \theta_0) \in \Pi T_{x_0} M$

$$S(\gamma, \theta) = S_0(x_0, \theta_0; \boldsymbol{y}, \boldsymbol{\eta}) + \text{ higher order terms in } y^{\mu}(t), \eta^{\mu}(t)$$

where

$$S_0(x_0, \theta_0; \boldsymbol{y}, \boldsymbol{\eta})$$
$$= \frac{1}{2} \int_0^1 \left(\dot{y}^{\mu}(t) \dot{y}^{\mu}(t) - \tilde{\mathrm{R}}_{\mu\nu}(x_0)\, \dot{y}^{\mu}(t) y^{\nu}(t) - \dot{\eta}^{\mu}(t) \eta^{\mu}(t) \right) dt, \tag{2.12}$$

[04] In Chapter 6 we considered the case of $M = \mathbb{R}^n$ with the standard Euclidean metric.

[5] This is the geometer's definition of the $\hat{A}$-genus; in topology one replaces R by $(2\pi i)^{-1}$R.

and

$$\tilde{\mathrm{R}}_{\mu\nu}\left(x_0\right)=\frac{1}{2}R_{\mu\nu\rho\sigma}\left(x_0\right)\theta_0^\rho\theta_0^\sigma.$$

Now using property (2.6) in Section 2.2 of Chapter 6 (where $m=\hbar=1$ and $T=1$), formula (4.10) in Section 4.3 of Chapter 7, and performing Gaussian integration, we get

$$\begin{aligned}\int_{\mathcal{L}(M)}e^{-S}&=(2\pi)^{-\frac{n}{2}}\int_{\Pi TM}\left(\int_{\mathcal{N}(\Pi TM)}e^{-S_0(x_0,\theta_0;\boldsymbol{y},\boldsymbol{\eta})}\mathscr{D}\boldsymbol{y}\mathscr{D}\boldsymbol{\eta}\right)d\boldsymbol{x}_0d\boldsymbol{\theta}_0\\&=(2\pi)^{-\frac{n}{2}}\int_{\Pi TM}\det{}'\left(-D^2\delta_{\mu\nu}-\tilde{\mathrm{R}}_{\mu\nu}\left(x_0,\theta_0\right)D\right)^{-\frac{1}{2}}d\boldsymbol{x}_0d\boldsymbol{\theta}_0\end{aligned}$$

where we have also used formula (4.12) in Section 4.3 of Chapter 7. Since $\tilde{\mathrm{R}}=\left\{\tilde{\mathrm{R}}_{\mu\nu}\right\}_{\mu,\nu=1}^{n}$ is a skew-symmetric matrix with even matrix elements, there is an orthogonal matrix C of determinant 1 such that

$$C\tilde{\mathrm{R}}C^{-1}=\begin{pmatrix}0&r_1&\cdots&0&0\\-r_1&0&\cdots&0&0\\\vdots&\vdots&\ddots&\vdots&\vdots\\0&0&\cdots&0&r_m\\0&0&\cdots&-r_m&0\end{pmatrix},\quad m=\frac{n}{2}.$$

It is easy to see that second order matrix differential operators

$$-D^2I_2+\begin{pmatrix}0&-r\\r&0\end{pmatrix}D\quad\text{and}\quad-D^2I_2+\begin{pmatrix}-ir&0\\0&ir\end{pmatrix}D$$

where I_2 is the 2×2 identity matrix, have the same spectrum. Using formula (3.5) in Section 3.2 of Chapter 6 with $\omega=\pm ir_k$, we get

$$\begin{aligned}\det{}'\left(-D^2\delta_{\mu\nu}-\tilde{\mathrm{R}}_{\mu\nu}D\right)&=\prod_{k=1}^{m}\det{}'\left(-D^2I_2+\begin{pmatrix}0&-r_k\\r_k&0\end{pmatrix}D\right)\\&=\prod_{k=1}^{m}\det{}'\left(-D^2-ir_kD\right)\det{}'\left(-D^2+ir_kD\right)\\&=\prod_{k=1}^{m}\left(\frac{\sin r_k/2}{r_k/2}\right)^2=\det\left(\frac{\sin\tilde{\mathrm{R}}/2}{\tilde{\mathrm{R}}/2}\right)\\&=j(i\tilde{\mathrm{R}})\end{aligned}$$

Therefore, using the identification $C^\infty(\Pi TM)\simeq\mathcal{A}^\bullet(M)$ we finally obtain

$$\begin{aligned}\int_{\mathcal{L}(M)}e^{-S}&=(2\pi)^{-\frac{n}{2}}\int_{\Pi ITM}j(i\tilde{\mathrm{R}}(x,\theta))^{-\frac{1}{2}}d\boldsymbol{x}d\boldsymbol{\theta}\\&=(2\pi i)^{-\frac{n}{2}}\int_M\hat{A}(M)\end{aligned}$$

Remark. Using formulas (2.6) in Section 2.2 of Chapter 6 and (4.10) in Section 4.3 of Chapter 7, we see that the same result holds for the space $\mathcal{L}_I(M)$ of loops on M parametrized by the interval $I=[0,T]$,

$$\int_{\Pi T\mathcal{L}_I(M)}e^{-\frac{1}{2}\int_0^T\left(\|\dot\gamma(t)\|^2+\left\langle\boldsymbol{\theta}(t),\nabla_{\dot\gamma(t)}\boldsymbol{\theta}(t)\right\rangle\right)dt}\mathscr{D}\boldsymbol{x}\mathscr{D}\boldsymbol{\theta}=(2\pi i)^{-\frac{n}{2}}\int_M\hat{A}(M).$$

Problem 2.3. Derive formula (2.8).
Problem 2.4. Derive formulas (2.11) and (2.12).
Problem 2.5. Justify the arguments in the "proof" of Theorem 2.3. (Hint: See the references in Section 7.)

26.1.4 Classical mechanics on supermanifolds

As was mentioned in Chapter 4, spin is a pure quantum notion which has no classical analog, and the same applies to fermion systems, considered in Chapter 7. However, one can formally consider particles with anticommuting coordinates and formulate classical mechanics on supermanifolds. Though such systems have no physical interpretation [6], their formal quantization yields fermion systems. This allows us to interpret particles with odd degrees of freedom as semi-classical limit of fermions.

3.1. Functions with anticommuting values.

Any smooth map $f : M \to N$ of smooth manifolds M and N gives rise to a Frchet algebra homomorphism

$$f^* : C^\infty(N) \to C^\infty(M)$$

where $f^*(\varphi) = \varphi \circ f$ for $\varphi \in C^\infty(N)$. Conversely, any Frchet algebra homomorphism $F : C^\infty(N) \to C^\infty(M)$ is of this form for some smooth map $f : M \to N$.

By definition, a map (morphism) between supermanifolds X and Y is a homomorphism of superalgebras

$$F : C^\infty(Y) \to C^\infty(X)$$

where $C^\infty(X)$ and $C^\infty(Y)$ are commutative superalgebras of global sections of corresponding structure sheaves $\mathcal{O}_X$ and $\mathcal{O}_Y$ (see Section 1). We will denote by $\mathrm{Map}(X, Y)$ the space of all maps between supermanifolds X and Y. The simplest cases are the following.

1. $X = \mathbb{R}^{0|1}$ - odd one-dimensional supermanifold, and $Y = M$ - an ordinary (even) manifold.
2. $X = \mathbb{R}$ (or S^1 and $I = [t_0, t_1]$) - even one-dimensional manifold, and $Y = \mathbb{R}^{0|n}$ - odd n-dimensional coordinate vector space.

In the first case every homomorphism of superalgebras $F : C^\infty(M) \to \mathbb{R}[\theta]$ has the form

$$F(\varphi) = A(\varphi) + B(\varphi)\theta, \quad \varphi \in C^\infty(M)$$

where $A : C^\infty(M) \to \mathbb{R}$ is an $\mathbb{R}$-algebra homomorphism, and $B : C^\infty(M) \to C^\infty(M)$ is a derivation of the commutative algebra $C^\infty(M)$. By the GelfandNaimark theorem, there exists $x \in M$ such that $A(\varphi) = \varphi(x)$, and $B(\varphi) = d\varphi(v)$ where $v \in T_xM$. Thus every map $f : \mathbb{R}^{0|1} \to M$ is given by a point $(x, v) \in TM$.

However, in the second case we have a homomorphism of superalgebras

$$F : \mathbb{R}\left[\theta^1, ..., \theta^n\right] \to C^\infty(\mathbb{R})$$

and since the commutative algebra $C^\infty(\mathbb{R})$ contains no nilpotents,

$$F\left(\theta^1\right) = \cdots = F\left(\theta^n\right) = 0$$

[06] Classical mechanics, which describes physical phenomena at the macroscopic level, necessarily uses commuting coordinates.

This result is clearly unsatisfactory, since every map $\mathbb{R} \to \mathbb{R}^{0|n}$ is trivial: $\theta^k(t) = 0, k = 1, ..., n$. To remedy this situation, one should consider the analog of Grothendieck's functor of points from algebraic geometry. Namely, introduce an auxiliary Grassmann algebra $W = \mathbb{R}\left[\eta^1, ..., \eta^N\right]$ and consider the product [7] $W \times \mathbb{R}$ with the superalgebra of functions $C^\infty(\mathbb{R})\left[\eta^1, ..., \eta^N\right]$. The " W-points" of Map $\left(\mathbb{R}, \mathbb{R}^{0|n}\right)$ are defined by homomorphisms of commutative superalgebras

$$F : \mathbb{R}\left[\theta^1, ..., \theta^n\right] \to \mathbb{C}^\infty(\mathbb{R})\left[\eta^1, ..., \eta^N\right]$$

In this case it is customary to write

$$\theta^k(t) = F\left(\theta^k\right) = a_1^k(t)\eta^1 + \cdots + a_N^k(t)\eta^N, \quad k = 1, ..., n \tag{3.1}$$

where real-valued $a_1^k(t), ..., a_N^k(t) \in C^\infty(\mathbb{R})$. It is convenient to think of $\theta^k(t)$ as smooth functions of variable t with anticommuting values, and define

$$\dot{\theta}^k(t) = \dot{a}_1^k(t)\eta^1 + \cdots + \dot{a}_N^k(t)\eta^N \tag{3.2}$$

where the dot stands for the derivative. To emphasize that Grassmann variables $\theta^k(t)$ are "real-valued", we will always assume that W is a set of fixed points in a Grassmann algebra with involution over $\mathbb{C}$, so that

$$\bar{\theta}^k(t) = \theta^k(t), \quad k = 1, ..., n$$

In the same way one defines W-points of Map $\left(S^1, \mathbb{R}^{0|n}\right)$ and Map $\left(I, \mathbb{R}^{0|n}\right)$.

Remark. This definition of the space of maps Map $\left(I, \mathbb{R}^{0|n}\right)$ (and also of the spaces Map $\left(\mathbb{R}, \mathbb{R}^{0|n}\right)$ and Map $\left(S^1, \mathbb{R}^{0|n}\right)$) is motivated by the definition used by physicists, who introduce an infinite-dimensional auxiliary Grassmann algebra W, so that for every t the values $\theta^k(t)$ are "independent real Grassmann variables".

Remark. One can also define functions on the space Map $\left(I, \mathbb{R}^{0|n}\right)$ - the functionals of functions with anticommuting values $\theta^k(t)$. Thus for the simplest example of the quadratic functional

$$S(\theta) = \frac{i}{2}\int_{t_0}^{t_1} \theta(t)\dot{\theta}(t)dt, \tag{3.3}$$

where we put $n = 1$ and $\theta^1(t) = \theta(t)$, using (3.1)-(3.2) we obtain

$$S(\theta) = \frac{i}{2}\int_{t_0}^{t_1} \left(a_k(t)\dot{a}_l(t) - \dot{a}_k(t)a_l(t)\right) dt\eta^k\eta^l \in \mathbb{R}\left[\eta^1, ..., \eta^N\right].$$

Here the factor $i = \sqrt{-1}$ ensures that $i\eta^k\eta^l$ are real Grassmann elements, i.e., $\overline{i\eta^k\eta^l} = -i\eta^l\eta^k = i\eta^k\eta^l$. In general, the space of "functions" on Map $\left(I, \mathbb{R}^{0|n}\right)$ is $\Lambda^\bullet\left(\text{Map}\left(I, \mathbb{R}^n\right)^*\right) \otimes W$, where Map $\left(I, \mathbb{R}^n\right)^*$ is the (topological) dual to the vector space Map $\left(I, \mathbb{R}^n\right)$, and W is a Grassmann algebra with infinitely many generators.

Vector fields with anticommuting values are naturally associated with the path space of a smooth manifold M. Namely, let

$$P_I(M) = \{\gamma : I \to M\},$$

where $I = [t_0, t_1]$, be the space of smooth parametrized paths in M. Consider the supermanifold ΠTM (see Section 1), and for every $\gamma \in P_I(M)$ let $\gamma^*(\Pi TM)$ be the pullback bundle

[07] Geometrically this corresponds to the family of spaces parametrized by W.

over I. By definition, a vector field with anticommuting values $\theta(t)$ is a section of $\gamma^*(\Pi TM)$ over I. In local coordinates $\boldsymbol{x} = (x^1, ..., x^n)$,

$$\boldsymbol{\theta}(t) = \theta^\mu(t)\frac{\partial}{\partial x^\mu} \in \Pi T_{\gamma(t)}M.$$

Thus

$$\Pi TP_I(M) = \{(\gamma, \theta) : \gamma \in P_I(M), \theta \in \Gamma\left(I, \gamma^*(\Pi TM)\right)\}.$$

Problem 3.1. Show that $S \in \Lambda^\bullet\left(\mathrm{Map}(I, \mathbb{R})^*\right) \otimes W$, where S is the quadratic functional given by (3.3).

3.2. Classical systems. Here we consider the basic examples of classical systems on supermanifolds.

Example 3.1 (Free classical particle of spin $\frac{1}{2}$). The configuration space is the supermanifold $\Pi T\mathbb{R}^3 \simeq \mathbb{R}^{3|3}$ - the tangent bundle to $\mathbb{R}^3$ with reversed parity of the fibers, with even and odd coordinates $\boldsymbol{x} = (x^1, x^2, x^3)$ and $\boldsymbol{\theta} = (\theta^1, \theta^2, \theta^3)$. The action functional $S : \Pi TP_I\left(\mathbb{R}^3\right) \to W$, where W is
some auxiliary Grassmann algebra, is defined by

$$\begin{aligned} S(\boldsymbol{x}(t), \boldsymbol{\theta}(t)) &= \int_{t_0}^{t_1} L(\boldsymbol{x}(t), \dot{\boldsymbol{x}}(t), \boldsymbol{\theta}(t))dt \\ &= \frac{1}{2}\int_{t_0}^{t_1} \left(m\dot{\boldsymbol{x}}^2 + i\boldsymbol{\theta}\dot{\boldsymbol{\theta}}\right)dt, \quad (\boldsymbol{x}(t), \boldsymbol{\theta}(t)) \in \Pi TP_I\left(\mathbb{R}^3\right) \end{aligned} \tag{3.4}$$

Here

$$L(\boldsymbol{x}(t), \dot{\boldsymbol{x}}(t), \boldsymbol{\theta}(t)) = \frac{1}{2}\left(m\dot{\boldsymbol{x}}^2(t) + i\boldsymbol{\theta}(t)\dot{\boldsymbol{\theta}}(t)\right)$$

is the Lagrangian function, which is real-valued since

$$\overline{i\boldsymbol{\theta}(t)\dot{\boldsymbol{\theta}}(t)} = -i\dot{\boldsymbol{\theta}}(t)\boldsymbol{\theta}(t) = i\boldsymbol{\theta}(t)\dot{\boldsymbol{\theta}}(t)$$

As in Section 1.2 of Chapter 1, we readily derive classical equations of motion as the following Euler-Lagrange equations:

$$\ddot{\boldsymbol{x}}(t) = 0 \quad \text{and} \quad \dot{\boldsymbol{\theta}}(t) = 0$$

Canonically conjugated momenta [8] are defined by

$$p^k = \frac{\partial L}{\partial \dot{x}^k} = m\dot{x}^k \quad \text{and} \quad \pi^k = \frac{\partial}{\partial \dot{\theta}^k}L = -\frac{i}{2}\theta^k, \quad k = 1, 2, 3$$

and the Hamiltonian function H is given by the Legendre transformation,

$$H = \boldsymbol{p}\dot{\boldsymbol{x}} + \dot{\boldsymbol{\theta}}\boldsymbol{\pi} - L = \frac{\boldsymbol{p}^2}{2m}$$

In agreement with classical equations of motion $\dot{\boldsymbol{\theta}}(t) = 0$, the Hamiltonian H does not depend on the odd variables. The phase space is a supermanifold $\mathbb{R}^{6|3}$ with real coordinates $\boldsymbol{p}, \boldsymbol{x}, \boldsymbol{\theta}$ and the symplectic form

$$\omega = d\boldsymbol{p} \wedge d\boldsymbol{x} - \frac{i}{2}d\boldsymbol{\theta}d\boldsymbol{\theta}$$

In accordance with Section 2.2 of Chapter 7, Poisson brackets between the odd variables are given by

$$\left\{\theta^k, \theta^l\right\} = i\delta^{kl}, \quad k, l = 1, 2, 3 \tag{3.5}$$

Poisson brackets satisfy the following involution property:

$$\overline{\{f_1, f_2\}} = (-1)^{|f_1||f_2|} \left\{\bar{f}_1, \bar{f}_2\right\}, \quad f_1, f_2 \in \mathbb{C}\left[\theta^1, \theta^2, \theta^3\right]. \tag{3.6}$$

We will see in Section 5 that quantization of this system describes the free quantum particle of spin $\frac{1}{2}$.

Example 3.2 (Classical spin $\frac{1}{2}$ particle in constant magnetic field). This system is described by the configuration space $\mathbb{R}^{3|3}$ with real coordinates $\boldsymbol{x}, \boldsymbol{\theta}$ and Lagrangian function

$$L = \frac{1}{2}\left(m\dot{\boldsymbol{x}}^2(t) + i\boldsymbol{\theta}(t)\dot{\boldsymbol{\theta}}(t) - i(\boldsymbol{B} \times \boldsymbol{\theta})\boldsymbol{\theta}\right).$$

The corresponding phase space and symplectic form are the same as in the previous example, and the Hamiltonian function is

$$H = \frac{\boldsymbol{p}^2}{2m} + \frac{i}{2}(\boldsymbol{B} \times \boldsymbol{\theta})\boldsymbol{\theta} \tag{3.7}$$

We will see in Section 5 that quantization of the Hamiltonian (3.7) yields the Pauli Hamiltonian.

Example 3.3 (Free particle on $\mathbb{R}^{n|n}$). Generalizing Example 3.1, consider the configuration space $\Pi T\mathbb{R}^n \simeq \mathbb{R}^{n|n}$ - the tangent bundle to $\mathbb{R}^n$ with reversed parity of the fibers, with even and odd real coordinates $\boldsymbol{x} = (x^1, ..., x^n)$ and $\boldsymbol{\theta} = (\theta^1, ..., \theta^n)$. The Lagrangian function

$$L(\boldsymbol{x}(t), \dot{\boldsymbol{x}}(t), \boldsymbol{\theta}(t)) = \frac{1}{2}\left(m\dot{x}^\mu\dot{x}^\mu + i\theta^\mu\dot{\theta}^\mu\right) \tag{3.8}$$

yields the same Euler-Lagrange equations as in Example 3.1,

$$\ddot{\boldsymbol{x}} = 0 \quad \text{and} \quad \dot{\boldsymbol{\theta}} = 0.$$

The corresponding phase space is a supermanifold $\mathbb{R}^{2n|n}$ with real coordinates $\boldsymbol{p}, \boldsymbol{x}, \boldsymbol{\theta}$ and the symplectic form

$$\omega = d\boldsymbol{p} \wedge d\boldsymbol{x} - \frac{i}{2}d\boldsymbol{\theta}d\boldsymbol{\theta}$$

and the Hamiltonian function is

$$H = \frac{\boldsymbol{p}^2}{2m}$$

Example 3.4 (Free particle on ΠTM). Let (M, g) be a Riemannian manifold with Riemannian metric $g_{\mu\nu}dx^\mu dx^\nu$. Similar to the construction in Section 2.2, we consider the phase space ΠTM with the Lagrangian function

$$L = \frac{1}{2}\left(\|\dot{\boldsymbol{x}}\|^2 + i\left\langle\boldsymbol{\theta}, \nabla_{\dot{\boldsymbol{x}}}\boldsymbol{\theta}\right\rangle\right), \tag{3.9}$$

where $\nabla_{\dot{\boldsymbol{x}}}$ is a covariant derivative along the path $\boldsymbol{x}(t)$ (which is also customarily denoted by D/Dt), and $\boldsymbol{\theta}(t) \in \Pi T_x M$. The corresponding action functional is defined by

[08] Here the indices are raised by the standard Euclidean metric on $\mathbb{R}^3$.

$$S = \frac{1}{2}\int_{t_0}^{t_1} \left(\|\dot{\boldsymbol{x}}\|^2 + i \left\langle \theta, \nabla_{\dot{\boldsymbol{x}}} \boldsymbol{\theta} \right\rangle \right) dt$$

or in local coordinates $\boldsymbol{x} = (x^1, ..., x^n)$ on M,

$$\begin{aligned} S &= \frac{1}{2}\int_{t_0}^{t_1} g_{\mu\nu}(\boldsymbol{x}(t)) \left(\dot{x}^\mu \dot{x}^\nu + \theta^\mu \frac{D\theta^\nu}{Dt} \right) dt \\ &= \frac{1}{2}\int_{t_0}^{t_1} g_{\mu\nu}(\boldsymbol{x}(t)) \left(\dot{x}^\mu \dot{x}^\nu + \theta^\mu \dot{\theta}^\nu + \Gamma^\nu_{\lambda\rho}(\boldsymbol{x}(t)) \dot{x}^\lambda \theta^\mu \theta^\rho \right) dt \end{aligned}$$

We will see in the next section that this system describes a supersymmetric particle on a Riemannian manifold.

Problem 3.2. Develop Lagrangian and Hamiltonian formalisms for classical mechanics on supermanifolds.

Problem 3.3. Prove formula (3.6).

Problem 3.4. Show that Euler-Lagrange equations for the system with Lagrangian (3.9) are

$$g_{\lambda\mu} \frac{D\dot{x}^\mu}{Dt} = \frac{1}{2} R_{\lambda\rho\mu\nu} \dot{x}^\rho \theta^\mu \theta^\nu \quad \text{and} \quad \frac{D\theta^\mu}{Dt} = 0$$

- equations for a spinning particle in a gravitational field.

Problem 3.5. Describe the phase space and find the Hamiltonian function for Example 3.4.

26.1.5 Supersymmetry

The Lagrangian system considered in Example 3.3 in the previous section possesses remarkable symmetries.

4.1. Total angular momentum.

First of all, the Lagrangian (3.8) is obviously invariant with respect to the action of the orthogonal group $G = \mathrm{SO}(n)$

$$L(g \cdot \dot{\boldsymbol{x}}, g \cdot \boldsymbol{\theta}) = L(\dot{\boldsymbol{x}}, \boldsymbol{\theta}), \quad g \in G \tag{4.1}$$

The corresponding conserved quantity - the Noether charge $\boldsymbol{J} \in \mathfrak{g}^*$ - the dual space to the Lie algebra $\mathfrak{g} = \mathfrak{so}(n)$, can be obtained as follows (cf. the proof of Theorem 1.3 in Section 1.4 of Chapter 1).

Consider an infinitesimal change of even and odd coordinates

$$\boldsymbol{x}(t) \mapsto \tilde{\boldsymbol{x}}(t) = \boldsymbol{x}(t) + \delta\boldsymbol{x}(t), \quad \boldsymbol{\theta}(t) \mapsto \tilde{\boldsymbol{\theta}}(t) = \boldsymbol{\theta}(t) + \delta\boldsymbol{\theta}(t),$$

and using $\dot{\boldsymbol{\theta}}\delta\boldsymbol{\theta} = -\delta\boldsymbol{\theta}\dot{\boldsymbol{\theta}}$, compute $\delta L = L(\dot{\boldsymbol{x}} + \delta\dot{\boldsymbol{x}}, \boldsymbol{\theta} + \delta\boldsymbol{\theta}) - L(\dot{\boldsymbol{x}}, \boldsymbol{\theta})$ up to the second order terms in $\delta\boldsymbol{x}$ and $\delta\boldsymbol{\theta}$,

$$\begin{aligned} \delta L &= m\dot{\boldsymbol{x}}\delta\dot{\boldsymbol{x}} + \frac{i}{2}(\delta\boldsymbol{\theta}\dot{\boldsymbol{\theta}} + \boldsymbol{\theta}\delta\dot{\boldsymbol{\theta}}) \\ &= -m\ddot{\boldsymbol{x}}\delta\boldsymbol{x} + m\frac{d}{dt}(\dot{\boldsymbol{x}}\delta\boldsymbol{x}) + \frac{i}{2}(\delta\boldsymbol{\theta}\dot{\boldsymbol{\theta}} - \dot{\boldsymbol{\theta}}\delta\boldsymbol{\theta}) + \frac{i}{2}\frac{d}{dt}(\boldsymbol{\theta}\delta\boldsymbol{\theta}) \\ &= -m\ddot{\boldsymbol{x}}\delta\boldsymbol{x} + m\frac{d}{dt}(\dot{\boldsymbol{x}}\delta\boldsymbol{x}) + i\delta\boldsymbol{\theta}\dot{\boldsymbol{\theta}} + \frac{i}{2}\frac{d}{dt}(\boldsymbol{\theta}\delta\boldsymbol{\theta}). \end{aligned}$$

Thus on the solutions of Euler-Lagrange equations $\ddot{\boldsymbol{x}} = 0, \dot{\boldsymbol{\theta}} = 0$ we have

$$\delta L = \frac{d}{dt}\left(m\dot{\boldsymbol{x}}\delta\boldsymbol{x} + \frac{i}{2}\boldsymbol{\theta}\delta\boldsymbol{\theta}\right).$$

Now using (4.1) with $g = e^{\varepsilon u}$, where $\boldsymbol{u} = \{u^\mu_\nu\}^n_{\mu,\nu=1}$ is a skew-symmetric $n \times n$ matrix, we see that $\delta L = 0$ for $\delta x^\mu = \varepsilon u^\mu_\nu x^\nu$ and $\delta\theta^\mu = \varepsilon u^\mu_\nu \theta^\nu$. Choosing the standard basis in the space of skew-symmetric $n \times n$ matrices, we obtain that components

$$J^{\mu\nu} = m\left(x^\mu \dot{x}^\nu - x^\nu \dot{x}^\mu\right) - i\theta^\mu\theta^\nu \tag{4.2}$$

are integrals of motion:

$$\frac{d}{dt}J^{\mu\nu} = 0$$

on solutions of the Euler-Lagrange equations. In particular, for $n = 3$ we get

$$\begin{aligned} J^1 &:= J^{23} = M^1 - i\theta^2\theta^3, \\ J^2 &:= J^{31} = M^2 - i\theta^3\theta^1, \\ J^3 &:= J^{12} = M^3 - i\theta^1\theta^2, \end{aligned}$$

where M^1, M^2, M^3 are components of the angular momentum $\boldsymbol{M}$ of a particle in $\mathbb{R}^3$ (see Section 1.4 in Chapter 1). We will see in the next section that after quantization the vector $\boldsymbol{J} = (J^1, J^2, J^3)$ becomes the total angular momentum operator of a quantum particle of spin $\frac{1}{2}$ in $\mathbb{R}^3$.

Remark. In fact, the Lagrangian (3.8) is invariant under the action of $G \times G$ on $\mathbb{R}^{n|n}$, so that both the angular momentum $m\left(x^\mu \dot{x}^\nu - x^\nu \dot{x}^\mu\right)$ in $\mathbb{R}^n$ and the "Grassmann angular momentum" $-i\theta^\mu\theta^\nu$ in $\mathbb{R}^{0|n}$ are conserved.

4.2. Supersymmetry transformation. It is quite remarkable that in addition to the symmetries discussed in the previous section, the Lagrangian (3.8) is also invariant under special transformations on $\mathbb{R}^{n|n}$ that mix even and odd coordinates. Namely, let $(\gamma(t), \boldsymbol{\theta}(t)) \in \Pi T P_I(\mathbb{R}^n)$, where $\boldsymbol{\theta}(t) \in \Pi T_\gamma P_I(\mathbb{R}^n)$ is a section over $I = [t_0, t_1]$ of the pull-back by γ of the tangent bundle of $T\mathbb{R}^n$ with reverse parity of the fibers,

$$\boldsymbol{\theta}(t) = \theta^\mu(t)\frac{\partial}{\partial x^\mu} \in \Pi T_{\gamma(t)} M$$

Consider the following infinitesimal change of coordinates which mixes even and odd variables:

$$\boldsymbol{x}(t) \mapsto \boldsymbol{x}(t) + \delta_\varepsilon \boldsymbol{x}(t) \quad \text{and} \quad \boldsymbol{\theta}(t) \mapsto \boldsymbol{\theta}(t) + \delta_\varepsilon \boldsymbol{\theta}(t), \tag{4.3}$$

where

$$\delta_\varepsilon \boldsymbol{x}(t) = i\varepsilon\boldsymbol{\theta}(t) \in T_{\boldsymbol{x}(t)}\mathbb{R}^n \quad \text{and} \quad \delta_\varepsilon\boldsymbol{\theta}(t) = -m\varepsilon\dot{\boldsymbol{x}}(t) \in \Pi T_{\boldsymbol{x}(t)}\mathbb{R}^n \tag{4.4}$$

and ε is an odd real element. Then for

$$\delta_\varepsilon L = L\left(\boldsymbol{x} + \delta_\varepsilon\boldsymbol{x}, \boldsymbol{\theta} + \delta_\varepsilon\boldsymbol{\theta}\right) - L(\boldsymbol{x}, \boldsymbol{\theta})$$

we obtain

$$\begin{aligned}\delta_\varepsilon L &= m\dot{\boldsymbol{x}}\delta_\varepsilon\dot{\boldsymbol{x}} + \frac{i}{2}\left(\delta_\varepsilon\boldsymbol{\theta}\dot{\boldsymbol{\theta}} + \boldsymbol{\theta}\delta_\varepsilon\dot{\boldsymbol{\theta}}\right)\\ &= im\dot{\boldsymbol{x}}\varepsilon\dot{\boldsymbol{\theta}} - \frac{im}{2}(\varepsilon\dot{\boldsymbol{x}}\dot{\boldsymbol{\theta}} + \boldsymbol{\theta}\varepsilon\ddot{\boldsymbol{x}})\\ &= \frac{im}{2}(\dot{\boldsymbol{x}}\varepsilon\dot{\boldsymbol{\theta}} + \varepsilon\boldsymbol{\theta}\ddot{\boldsymbol{x}})\\ &= \frac{im\varepsilon}{2}\frac{d}{dt}(\boldsymbol{\theta}\dot{\boldsymbol{x}}).\end{aligned}$$

Thus for periodic boundary conditions the action functional

$$S(\gamma,\theta) = \int_{t_0}^{t_1} L(\gamma(t),\boldsymbol{\theta}(t))dt$$

is invariant under the change of coordinates (4.3),

$$\delta_\varepsilon S(\gamma,\theta) = 0 \quad \text{for all periodic } (\gamma,\theta)\in \Pi TP_I(\mathbb{R}^n)$$

The infinitesimal transformation (4.3) is called the supersymmetry transformation.

Remark. We emphasize that invariance of the action under the supersymmetry transformations holds for all $(\gamma(t),\boldsymbol{\theta}(t))$ with periodic boundary conditions, and not only on equations of motion!

Introducing the quantity

$$Q = im\boldsymbol{\theta}\dot{\boldsymbol{x}} = i\boldsymbol{\theta}\boldsymbol{p} = i\theta^\mu p_\mu,$$

called the generator of supersymmetry (or the supercharge), we can summarize the above computation as

$$\delta_\varepsilon L = \frac{\varepsilon}{2}\frac{dQ}{dt}. \tag{4.5}$$

Another remarkable property is that the Lagrangian L can be recovered from the supercharge Q. Namely, the simple computation

$$\delta_\varepsilon Q = m\left(\delta_\varepsilon\boldsymbol{\theta}\dot{\boldsymbol{x}} + \boldsymbol{\theta}\delta_\varepsilon\dot{\boldsymbol{x}}\right) = m\varepsilon\left(-m\dot{\boldsymbol{x}}^2 - i\boldsymbol{\theta}\dot{\boldsymbol{\theta}}\right)$$

gives

$$-2mi\varepsilon L = \delta_\varepsilon Q \tag{4.6}$$

Using (3.5) we obtain

$$\{Q,Q\} = -i\boldsymbol{p}^2 = -2miH \tag{4.7}$$

which shows that the Hamiltonian H can also be recovered from the supercharge Q.

Remark. Geometrically, supersymmetry transformation is just an equivariant differential on the space $\mathcal{L}_I(\mathbb{R}^n)$ of free loops on $\mathbb{R}^n$ parametrized by the interval $I=[t_0,t_1]$, considered in Section 2.2 (for the interval $[0,1]$). Namely, set $m=1$ and consider the Wick rotation $t\mapsto -it$ to the Euclidean time, so that the sypersymmetry transformation (4.3)-(4.4) becomes

$$\delta_\varepsilon\boldsymbol{x}(t) = i\varepsilon\boldsymbol{\theta}(t), \quad \delta_\varepsilon\boldsymbol{\theta}(t) = -i\varepsilon\dot{\boldsymbol{x}}(t). \tag{4.8}$$

Now we immediately see that formulas (4.8) can be written as

$$\delta_\varepsilon\boldsymbol{x}(t) = i\varepsilon D\boldsymbol{x}(t) \quad \text{and} \quad \delta_\varepsilon\boldsymbol{\theta}(t) = i\varepsilon D\boldsymbol{\theta}(t),$$

where D is the equivariant differential (2.7),

$$D = \int_{t_0}^{t_1} \left(\theta^\mu(t) \frac{\delta}{\delta x^\mu(t)} - \dot{x}^\mu(t) \frac{\delta}{\delta \theta^\mu(t)} \right) dt,$$

which satisfies $D^2 = -\mathcal{L}_{\dot{\gamma}}$. The corresponding Euclidean supercharge Q coincides with the function β on $\Pi T\mathcal{L}(\mathbb{R}^n)$, given by formula (2.9), so that

$$Q = \int_{t_0}^{t_1} \theta^\mu(t) \dot{x}^\mu(t) dt$$

where we are using the standard Euclidean metric on $\mathbb{R}^n$. It follows from Lemma 2.2 that

$$DQ = -\int_{t_0}^{t_1} (\dot{\boldsymbol{x}}(t)\dot{\boldsymbol{x}}(t) + \boldsymbol{\theta}(t)\dot{\boldsymbol{\theta}}(t)) dt = -2S(\boldsymbol{x}(t), \boldsymbol{\theta}(t)),$$

where now S stands for the Euclidean action. The invariance of the action S under the supersymmetry transformation is the property that S is equivariantly closed, $DS = 0$.

Problem 4.1. Verify that

$$[\delta_{\varepsilon_1}, \delta_{\varepsilon_2}] = 2i\varepsilon_1\varepsilon_2 \frac{d}{dt},$$

where $\varepsilon_1, \varepsilon_2$ are odd variables, and deduce from it formula (4.7).

4.3. Supersymmetric particle on a Riemannian manifold. The classical system with Lagrangian (3.9), considered in Example 3.4 in Section 3.2 , describes a supersymmetric particle on a Riemannian manifold (M, g). Namely, for $(\gamma, \theta) \in \Pi T P_I(M)$ define the supersymmetry transformation $\boldsymbol{x}(t) \mapsto \boldsymbol{x}(t) + \delta_\varepsilon \boldsymbol{x}(t)$ and $\boldsymbol{\theta}(t) \mapsto \boldsymbol{\theta}(t) + \delta_{\boldsymbol{\varepsilon}} \boldsymbol{\theta}(t)$, in local coordinantes $\boldsymbol{x}(t)$ and $\boldsymbol{\theta}(t)$, by the same formula (4.4),

$$\delta_\varepsilon \boldsymbol{x}(t) = i\varepsilon \boldsymbol{\theta}(t) \in \Pi T_{\gamma(t)} M, \quad \delta_\varepsilon \boldsymbol{\theta}(t) = -m\varepsilon \dot{\boldsymbol{x}}(t) \in \Pi T_{\gamma(t)} M, \tag{4.9}$$

where ε is an odd real element.

Lemma 4.1. Supersymmetry transformation (4.9) does not depend on the choice of local coordinates.

Proof. Let $\tilde{\boldsymbol{x}} = (\tilde{x}^1, ..., \tilde{x}^n)$ be another local coordinates on $M, \tilde{x}^\mu = f^\mu(\boldsymbol{x}), \mu = 1, ..., n$. Along the path $\gamma = \boldsymbol{x}(t)$,

$$\dot{\tilde{x}}^\mu(t) = \frac{\partial f^\mu}{\partial x^\nu}(\boldsymbol{x}(t)) \dot{x}^\nu(t) \quad \text{and} \quad \boldsymbol{\theta}(t) = \tilde{\theta}^\mu(t) \frac{\partial}{\partial \tilde{x}^\mu}$$

where

$$\tilde{\theta}^\mu(t) = \frac{\partial f^\mu}{\partial x^\nu}(\boldsymbol{x}(t)) \theta^\nu(t).$$

We have

$$\delta_\varepsilon \tilde{x}^\mu(t) = \frac{\partial f^\mu}{\partial x^\nu}(\boldsymbol{x}(t)) \delta_\varepsilon x^\nu(t) = i \frac{\partial f^\mu}{\partial x^\nu}(\boldsymbol{x}(t)) \varepsilon \theta^\nu(t) = i\varepsilon \tilde{\theta}^\mu(t),$$

and

$$\begin{aligned} \delta_\varepsilon \tilde{\theta}^\mu(t) &= \frac{\partial f^\mu}{\partial x^\nu}(\boldsymbol{x}(t)) \delta_\varepsilon \theta^\nu(t) + \frac{\partial^2 f^\mu}{\partial x^\nu \partial x^\sigma}(\boldsymbol{x}(t)) \delta_\varepsilon x^\sigma(t) \theta^\nu(t) \\ &= -m\varepsilon \frac{\partial f^\mu}{\partial x^\nu}(\boldsymbol{x}(t)) \dot{x}^\nu(t) + i\varepsilon \frac{\partial^2 f^\mu}{\partial x^\nu \partial x^\sigma}(\boldsymbol{x}(t)) \theta^\sigma(t) \theta^\nu(t) \\ &= -m\varepsilon \dot{\tilde{x}}^\mu(t), \end{aligned}$$

since $\theta^\mu(t)$ anticommute.
As in the previous section, we define the supercharge Q by

$$Q(t) = im\langle \dot{\boldsymbol{x}}(t), \boldsymbol{\theta}(t)\rangle$$

The main result of this section is the following statement.
Proposition 4.1. Under the supersymmetry transformation (4.9),

$$\delta_\varepsilon Q = -2mi\varepsilon L \tag{4.10}$$

where

$$L = \frac{m}{2}\|\dot{\boldsymbol{x}}\|^2 + \frac{i}{2}\langle \boldsymbol{\theta}, \nabla_{\dot\gamma}\boldsymbol{\theta}\rangle \tag{4.11}$$

is the Lagrangian of a free particle on Π TM. Also

$$\delta_\varepsilon L = \frac{\varepsilon}{2}\frac{dQ}{dt}. \tag{4.12}$$

Proof. The derivation of (4.10) is a straightforward computation using formula (2.11). Formula (4.12) is proved by another computation, similar to the one used to prove (4.5) in the previous section.

Corollary 4.1. The action functional

$$S(\gamma,\theta) = \int_{t_0}^{t_1} L(\gamma(t), \boldsymbol{\theta}(t))dt$$

is invariant under the supersymmetry transformations,

$$\delta_\varepsilon S(\gamma,\theta) = 0 \quad \text{for all periodic } (\gamma,\theta) \in \Pi TP_I(M)$$

Remark. As for the example of a free particle on $\mathbb{R}^{n|n}$, considered in Section 4.2, the Euclidean version of the sypersymmetry transformation (4.9) corresponds to the equivariant differential (2.7) on the space $\boldsymbol{\mathcal{L}}_I(M)$ of free loops on M parametrized by the interval $I = [t_0, t_1]$. The corresponding Euclidean supercharge Q (for $m = 1$) coincides with the function β on $\Pi T\boldsymbol{\mathcal{L}}_I(M)$ given by formula (2.9), and Proposition 4.1 reduces to the statements that $DQ = -2S$ and $DS = 0$, where S is the Euclidean action, proved in Lemma 2.2.

Problem 4.2. Prove all the formulas in this section.
Problem 4.3 (Superfield formalism). For $(\gamma,\theta) \in \Pi TM$ define the superfield by $X(t) = \boldsymbol{x}(t) + \eta\boldsymbol{\theta}(t)$, where η is an auxiliary Grassmann variable, and let $\mathcal{D} = \frac{\partial}{\partial\eta} - \eta\frac{\partial}{\partial t}$. Show that

$$\int g_{\mu\nu}(X(t))\dot X(t)\mathcal{D}(X)(t)dtd\eta = -\int_{t_0}^{t^1}\left(\|\dot{\boldsymbol{x}}\|^2 + \langle\boldsymbol{\theta}, \nabla_{\dot\gamma}\boldsymbol{\theta}\rangle\right)dt$$

- twice the Euclidean action of a supersymmetric particle on a Riemannian manifold M.

26.1.6 Quantum mechanics on supermanifolds

Here we describe quantum systems which correspond to classical systems in Section 3.2. According to the correspondence principle (see Section 2 of Chapter 2), for quantization of even coordinates we replace Poisson brackets $\{,\}byi[,], wherei = \sqrt{-1}$ and $[,]isthecommutator$[9]. For quantization of odd coordinates, in accordance with Section 1 of Chapter 7, we replace corresponding Poisson brackets by $i[,]_+$, where $[,]_+$is the anticommutator.

Example 5.1 (Quantum particle of spin $\frac{1}{2}$). The corresponding phase space is a supermanifold $\mathbb{R}^{6|3}$ with even coordinates $\boldsymbol{p} = (p_1, p_2, p_3)$ and $\boldsymbol{x} = (x_1, x_2, x_3)$, and odd coordinates ${}^{10}\boldsymbol{\theta} = (\theta_1, \theta_2, \theta_3)$, with canonical Poisson brackets

$$\{p_\mu, x_\nu\} = \delta_{\mu\nu} \quad \text{and} \quad \{\theta_\mu, \theta_\nu\} = i\delta_{\mu\nu}, \quad \mu, \nu = 1, 2, 3$$

Quantum operators $\boldsymbol{P} = (P_1, P_2, P_3)$ and $\boldsymbol{Q} = (Q_1, Q_2, Q_3)$, which correspond to canonical coordinates $\boldsymbol{p}$ and $\boldsymbol{x}$, satisfy Heisenberg commutation relations (see Section 2.1 of Chapter 2), while operators $\boldsymbol{\Theta} = (\Theta_1, \Theta_2, \Theta_3)$, which correspond to the anticommuting coordinates $\boldsymbol{\theta}$, satisfy the following anticommutation relations:

$$[\Theta_\mu, \Theta_\nu]_+ = \delta_{\mu\nu} I, \quad \mu, \nu = 1, 2, 3. \tag{5.1}$$

Since operators $\sqrt{2}\Theta_\mu$ define a representation of a Clifford algebra C_3, the only irreducible realization of (5.1) is given by

$$\Theta_\mu = \frac{1}{\sqrt{2}}\sigma_\mu, \quad \mu = 1, 2, 3 \tag{5.2}$$

where σ_μ are Pauli matrices (see Section 1.1 of Chapter 4). Thus the Hilbert space of the system is $\mathscr{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$ - the Hilbert space of a quantum particle of spin $\frac{1}{2}$ - and the Hamiltonian operator is

$$H = \frac{\boldsymbol{P}^2}{2m}$$

Using (5.2) and the multiplication table of Pauli matrices, we obtain the following form for quantum Noether integrals of motion (4.2):

$$J = M + S$$

where $\boldsymbol{M}$ is the angular momentum operator (see Section 3.1 of Chapter 3), and $\boldsymbol{S} = \frac{1}{2}\boldsymbol{\sigma}$. Thus $\boldsymbol{J}$ is the total angular momentum operator of a quantum spin $\frac{1}{2}$ particle (see Section 1.2 of Chapter 4).

Example 5.2 (Quantum spin $\frac{1}{2}$ particle in constant magnetic field). The Hilbert space is the same as in the previous example, while the Hamiltonian operator which corresponds to (3.7) takes the form

$$H = \frac{\boldsymbol{P}^2}{2m} + \frac{i}{2}(\boldsymbol{B} \times \boldsymbol{\Theta})\boldsymbol{\Theta} = \frac{\boldsymbol{P}^2}{2m} - \frac{\mathbf{B} \cdot \boldsymbol{\sigma}}{2}.$$

Thus operator H is the Pauli Hamiltonian with total magnetic moment $\mu = \frac{1}{2}$ (see Section 2.1 of Chapter 4).

Example 5.3 (Supersymmetric quantum particle on $\mathbb{R}^n$). The phase space is a supermanifold $\mathbb{R}^{2n|n}$ with even coordinates $\boldsymbol{p} = (p_1, ..., p_n)$ and $\boldsymbol{x} = (x_1, ..., x_n)$, and odd coordinates $\boldsymbol{\theta} = (\theta_1, ..., \theta_n)$, with canonical Poisson brackets

$$\{p_\mu, x_\nu\} = \delta_{\mu\nu} \quad \text{and} \quad \{\theta_\mu, \theta_\nu\} = i\delta_{\mu\nu}, \quad \mu, \nu = 1, ..., n$$

Quantum operators $\boldsymbol{P} = (P_1, ..., P_n)$ and $\boldsymbol{Q} = (Q_1, ..., Q_n)$, which correspond to canonical coordinates $\boldsymbol{p}$ and $\boldsymbol{x}$, satisfy Heisenberg commutation relations, and operators $\Theta = (\Theta_1, ..., \Theta_n)$, which correspond to the anticommuting coordinates $\boldsymbol{\theta}$, satisfy the following anticommutation relations:

[09] Here we put $h = 1$.

[10] Here it is convenient to lower all indices by the standard Euclidean metric on $\mathbb{R}^3$.

$$[\Theta_\mu, \Theta_\nu]_+ = \delta_{\mu\nu} I, \quad \mu, \nu = 1, ..., n \tag{5.3}$$

The operators $\sqrt{2}\Theta^\mu$ define a representation of a Clifford algebra C_n. When n is even, the only irreducible realization of (5.3) is

$$\Theta_\mu = \frac{1}{\sqrt{2}}\gamma_\mu$$

where γ_μ are operators in $\mathscr{H}_F = (\mathbb{C}^2)^{\otimes d}, d = \frac{n}{2}$, given by formulas (1.12)(1.13) in Section 1.2 of Chapter 7 . For odd n, operators γ act in $(\mathbb{C}^2)^{\otimes d}$, where $d = \left[\frac{n}{2}\right]$ (see Problem 1.4 in Section 1.2 of Chapter 7). In both cases, the Hilbert space of the system is $\mathscr{H} = L^2(\mathbb{R}^n) \otimes \mathscr{H}_F = L^2(\mathbb{R}^n) \otimes \mathbb{C}^{2^d}$, the Hamiltonian operator is given by

$$H = \frac{\boldsymbol{P}^2}{2m}$$

and quantum Noether integrals of motion are

$$J_{\mu\nu} = Q_\mu P_\nu - Q_\nu P_\mu - i\Theta_\mu\Theta_\nu$$

Quantization of the supercharge gives the operator

$$Q = i\Theta_\mu P_\mu = \frac{i}{\sqrt{2}}\gamma_\mu P_\mu = \frac{1}{\sqrt{2}}\gamma_\mu\frac{\partial}{\partial x_\mu} = \frac{1}{\sqrt{2}}\ \not{\partial} \tag{5.4}$$

where

$$\not{\partial} = \gamma_\mu\frac{\partial}{\partial x_\mu}$$

is the Dirac operator on $\mathbb{R}^n$. The Dirac operator is skew-adjoint in $\mathscr{H}$,

$$\not{\partial}^* = -\ \not{\partial}.$$

When n is even, decomposition $\mathscr{H}_F = \mathscr{H}_F^+ \oplus \mathscr{H}_F^-$ into the subspaces of positive and negative chirality spinors (see Section 1.2 of Chapter 7) gives decomposition

$$\mathscr{H} = \mathscr{H}_+ \oplus \mathscr{H}_-, \qquad \text{where} \qquad \mathscr{H}_\pm = L^2(\mathbb{R}^n) \otimes \mathscr{H}_F^\pm$$

and using that $\gamma_\mu\left(\mathscr{H}_F^+\right) = \mathscr{H}_F^-$ (see Section 1.2 of Chapter 7), we can represent the Dirac operator in the following 2×2 block-matrix form:

$$\not{\partial} = \begin{pmatrix} 0 & -\ \not{\partial}_+^* \\ \not{\partial}\partial_+ & 0 \end{pmatrix}$$

Here the operator $\not{\partial}: \mathscr{H}_+ \to \mathscr{H}_-$ is called the chiral Dirac operator. We have

$$[Q, Q]_+ = 2Q^2 = \not{\partial}^2 = -2mH$$

so that $2mH$ is the Dirac Laplacian $-\ \not{\partial}^2$. In matrix form,

$$2mH = \begin{pmatrix} \ddot{\not{\partial}}_+^* \not{\partial}_+ & 0 \\ 0 & \not{\partial}_+ \ddot{\not{\partial}}_+^* \end{pmatrix}$$

Example 5.4 (Supersymmetric quantum particle on Riemannian manifold). We have seen in Example 2.4 in Section 2.4 of Chapter 2 that though for a free quantum particle on a Riemannian manifold (M, g) it is not possible to construct operators $\boldsymbol{P}$ and $\boldsymbol{Q}$ which correspond to standard

local coordinates $(\boldsymbol{p}, \boldsymbol{x})$ on T^*M, the Hamiltonian operator H is well defined as the Laplace-Beltrami operator of the Riemannian metric. It is remarkable
that consistent quantization of a supersymmetric particle requires M to be a spin manifold, and for even $n = \dim M$ the corresponding supercharge operator Q coincides with the Dirac operator!

Namely, let $\mathrm{Spin}(n)$ be the spin group: connected, simply connected Lie group which is a double cover of $\mathrm{SO}(n)$. The oriented Riemannian manifold (M, g) of dimension n is said to have a spin structure (and is called a spin manifold) if the bundle $\mathrm{SO}(M)$ of oriented orthonormal frames over M principal $\mathrm{SO}(n)$-bundle - can be extended to the principal $\mathrm{Spin}(n)$-bundle $\mathrm{Spin}(M)$. This is equivalent to the condition that for some open covering $M = \bigcup_{\alpha\in A} U_\alpha$ transition functions $t_{\alpha\beta} : U_\alpha \cap U_\beta \to \mathrm{SO}(n)$ of a tangent bundle TM can be lifted to the transition functions $\tau_{\alpha\beta} : U_\alpha \cap U_\beta \to \mathrm{Spin}(n)$; $t_{\alpha\beta} = \rho(\tau_{\alpha\beta})$, where $\rho : \mathrm{Spin}(n) \to \mathrm{SO}(n)$ is the canonical projection. The manifold M is a spin manifold if and only if its second Stieffel-Whitney class $w_2 \in H^2(M, \mathbb{Z}_2)$ vanishes; in this case different spin structures are parametrized by $H^1(M, \mathbb{Z}_2) \simeq \mathrm{Hom}(\pi_1(M), \mathbb{Z}_2)$, where $\pi_1(M)$ is the fundamental group of M. For even $n = 2d$, the irreducible representation ρ of the Clifford algebra C_n in $\mathscr{H}_F \simeq \mathbb{C}^{2^d}$ (see Section 1.2 of Chapter 7) defines unitary representation R of the spin group $\mathrm{Spin}(n)$ in $\mathscr{H}_F$, which commutes with the parity operator Γ. By definition, the spinor bundle $\mathcal{S}$ on an evendimensional spin manifold M is a Hermitian vector bundle associated with the principal $\mathrm{Spin}(n)$-bundle $\mathrm{Spin}(M)$ by the unitary representation R. In other words, $\mathcal{S}$ is a complex vector bundle with the transition functions $R(\tau_{\alpha\beta}) : U_\alpha \cap U_\beta \to \mathrm{U}\left(2^d\right)$, where $\mathrm{U}\left(2^d\right)$ is the group of unitary $2^d \times 2^d$ matrices. Decomposition of vector spaces $\mathscr{H}_F = \mathscr{H}_F^+ \oplus \mathscr{H}_F^-$ defines the decomposition

$$\mathcal{S} = \mathcal{S}_+ \oplus \mathcal{S}_-$$

of the spinor bundle $\mathcal{S}$ into the bundles $\mathcal{S}_+$and $\mathcal{S}_-$ of positive and negative chirality spinors.

The Dirac operator $\not{\partial} : C^\infty(M, \mathcal{S}) \to C^\infty(M, \mathcal{S})$ of the even-dimensional spin manifold M is defined as follows. Let $\nabla^{\mathcal{S}}$ be the connection on the spinor bundle $\mathcal{S}$ induced by the Levi-Civita connection in the tangent bundle TM. Then in the coordinate chart $U \subset M$ with local coordinates $\boldsymbol{x} = (x^1, ..., x^n)$ we have

$$\not{\partial} = \gamma^\mu(\boldsymbol{x})\nabla_\mu^{\mathcal{S}} \tag{5.5}$$

where $\nabla_\mu^{\mathcal{S}}$ is the covariant derivative with respect to the vector field $\frac{\partial}{\partial x^\mu}$ over U, and $\gamma^\mu(\boldsymbol{x})$ are endomorphisms of the spinor bundle $\mathcal{S}$ over U satisfying

$$[\gamma^\mu(\boldsymbol{x}), \gamma^\nu(\boldsymbol{x})]_+ = 2g^{\mu\nu}(\boldsymbol{x})I \tag{5.6}$$

where I is the identity endomorphism. It is easy to show that there is an open covering $M = \bigcup_{\alpha\in A} U_\alpha$ such that $\gamma^\mu(\boldsymbol{x})$ exist over each U_α, and that local
expressions (5.5) give rise to a globally defined operator $\not{\partial}$: $C^\infty(M, \mathcal{S}) \to C^\infty(M, \mathcal{S})$. Equivalently, if $\xi \in C^\infty(M, \mathcal{S})$ is given by $\xi = \{\xi_\alpha\}_{\alpha\in A}, \xi_\alpha$: $U_\alpha \to \mathscr{H}_F$, where $\xi_\alpha = R(\tau_{\alpha\beta})\,\xi_\beta$ on $U_\alpha \cap U_\beta$, then

$$\not{\partial}_\alpha \xi_\alpha = R(\tau_{\alpha\beta})\ \not{\partial}_\beta \xi_\beta, \tag{5.7}$$

where $\not{\partial}$ is given by (5.5) for $U = U_\alpha$. We also have

$$\not{\partial} : C^\infty(M, \mathcal{S}_\pm) \to C^\infty(M, \mathcal{S}_\mp).$$

The Hermitian metric $\|\|_{\mathcal{S}}$ in the spinor bundle $\mathcal{S}$ and the Riemannian metric g on M allow us to define the Hilbert space $\mathscr{H}$ of square integrable global sections of $\mathcal{S}$,

$$\mathscr{H} = \left\{ \xi \in \Gamma(M, \mathcal{S}) : \|\xi\|^2 = \int_M \|\xi(x)\|^2_{\mathcal{S}} d\mu(x) < \infty \right\}.$$

Initially defined on $C^\infty(M, \mathcal{S})$, the Dirac operator extends to the skewadjoint operator in $\mathscr{H}$, which we continue to denote by $\not{\partial}$. As in the previous example, using the Hilbert space decomposition $\mathscr{H} = \mathscr{H}_+ \oplus \mathscr{H}_-$, we can represent the Dirac operator in the following 2×2 block-matrix form:

$$\not{\partial} = \begin{pmatrix} 0 & -\not{\partial}^*_+ \\ \not{\partial}_+ & 0 \end{pmatrix},$$

where $\partial_+ : \mathscr{H}_+ \to \mathscr{H}_-$is the chiral Dirac operator on a spin manifold M.

Remark. The Dirac operator from the previous example is the Dirac operator on the spin manifold $\mathbb{R}^n$ with the standard Euclidean metric; the corresponding spinor bundle is a trivial Hermitian vector bundle $\mathbb{R}^n \times \mathscr{H}_F$.

The space of states of a quantum supersymmetric particle on a spin manifold (M, g) is the Hilbert space $\mathscr{H}$ of square-integrable sections of the spinor bundle S over M. The corresponding supercharge operator Q and Hamiltonian operator H are given by the same formulas as in the previous example,

$$Q = \frac{1}{\sqrt{2}} \not{\partial} \quad \text{and} \quad [Q, Q]_+ = 2Q^2 = \not{\partial}^2 = -2mH.$$

The operator

$$2mH = \begin{pmatrix} \not{\partial}^*_+ \not{\partial}_+ & 0 \\ 0 & \not{\partial}_+ \not{\partial}^*_+ \end{pmatrix}$$

is the Dirac Laplacian on a spin manifold M.

Problem 5.1. Identify the spin group $\mathrm{Spin}(n)$ as a subgroup in the group of invertible elements of the Clifford algebra C_n.

Problem 5.2. Prove relations (5.7).

26.1.7 Atiyah-Singer index formula

Let M be an even-dimensional, oriented, compact spin manifold with the Riemannian metric g. Operators $\not{\partial}^*_+ \not{\partial}_+$and $\not{\partial}_+ \not{\partial}^*_+$ are, respectively, selfadjoint on Hilbert spaces $\mathscr{H}_+$and $\mathscr{H}_-$, and have pure point spectra consisting of non-negative eigenvalues of finite multiplicity with the only accumulation point at ∞. In particular, complex vector spaces $\ker \not{\partial}^*_+ \not{\partial}_+ = \ker \not{\partial}_+$and $\ker \not{\partial}_+ \not{\partial}^*_+ = \ker \not{\partial}^*_+$ are finite-dimensional, and we define the index $\mathrm{ind}\ \not{\partial}_+$of the chiral Dirac operator $\not{\partial}_+$by

$$\mathrm{ind}\ \not{\partial}_+ = \dim \ker \not{\partial}_+ - \dim \ker \not{\partial}^*_+.$$

We have the following basic result.

Theorem 6.1 (McKean-Singer). For every $T > 0$,

$$\mathrm{ind}\ \not{\partial}_+ = \mathrm{Tr}_s\, e^{T\not{\partial}^2} = \mathrm{Tr}\, e^{-T\not{\partial}^*_+ \not{\partial}_+} - \mathrm{Tr}\, e^{-T\not{\partial}_+ \not{\partial}^*_+}.$$

On the other hand, we have seen in Example 5.4 in the last section that $-\not{\partial}^2 = 2H$, where H is the Hamiltonian operator of free supersymmetric particle of mass $m = 1$ on the spin manifold M. Thus for every $T > 0$,

$$\mathrm{ind}\ \not{\partial}_+ = \mathrm{Tr}_s\, e^{-2TH}$$

In Section 2.2 of Chapter 6 and in Sections 4.2 and 4.3 of Chapter 7 we developed a formalism for expressing traces and supertraces of the evolution operator in Euclidean time by path integrals. Using these results, we can, at a physical level of rigor, represent the supertrace $\mathrm{Tr}_s\, e^{-2TH}$ by the path integral

$$\mathrm{Tr}_s\, e^{-2TH} = \int_{\Pi T\mathcal{L}_I(M)} e^{-S_{\mathrm{E}}(\gamma,\theta)}\mathscr{D}\boldsymbol{x}\mathscr{D}\boldsymbol{\theta} \tag{6.1}$$

Here

$$S_{\mathrm{E}}(\gamma,\theta) = \frac{1}{2}\int_0^{2T}\left(\|\dot\gamma\|^2 + \langle\boldsymbol{\theta}(t), \nabla_{\dot\gamma}\boldsymbol{\theta}(t)\rangle\right)dt$$

is the Euclidean action of a supersymmetric particle on a Riemannian manifold M, obtained from the Lagrangian function (4.11) by replacing time t by the Euclidean time $-it$, and $\mathcal{L}_I(M)$ is the space of free loops on M parametrized by the interval $[0, 2T]$. When [11]$2T = 1$, the integral in (6.1) coincides with integral $\int_{\mathcal{L}(M)} e^{-S}$, considered in Section 2.2. Using Theorem 2.3, we obtain

$$\mathrm{ind}\ \not{\partial}_+ = \mathrm{Tr}_s\, e^{-H} = (2\pi i)^{-\frac{n}{2}}\int_M \hat{A}(M),$$

which is the celebrated Atiyah-Singer formula for the index of the Dirac operator on a spin manifold!

Remark. Integrating over Grassmann variables in (6.1), we obtain

$$\mathrm{Tr}_s\, e^{-H} = \int_{\mathcal{L}(M)} \mathrm{Pf}\,(\nabla_{\dot\gamma})\, d\mu_W \tag{6.2}$$

where $d\mu_W$ is the Wiener measure on the loop space $\mathcal{L}(M)$ associated with the Riemannian metric g on M. It can be shown that when M is a spin manifold, the Pfaffian $\mathrm{Pf}\,(\nabla_{\dot\gamma})$ of a covariant derivative operator along $\gamma \in \mathcal{L}(M)$ is a well-defined function on $\mathcal{L}(M)$. Thus formula (6.2), as opposed to the local computation in the derivation of Theorem 2.3, captures global properties of the manifold M.

Problem 6.1. Prove the McKean-Singer theorem.

Problem 6.2. "Derive" formula (6.1). (Hint: See the references in the next section.)

27 Deeper Understanding of Quantum Mechanics

(I'll merge it with the part 2 later)

27.1 Construction of Quantum Mechanics (?)

(пока так раздел называется, посмотрим, мб назову иначе)

27.1.1 Gauges in Quantum Mechanics (??)

(пока так сказать мало что могу)

[011] According to a remark in Section 2.2, the same result holds for every $T > 0$.

О калибровочной инвариантности (???)

Нам известно, что волновая функция определена с точностью до глобальной фазы, так как она не влияет ни на интерференцию всех слагаемых, ни на модуль вероятности.

(?? честно, пока хз, что сказать про это с точки зрения квантмеха, повисит пока раздел)

вывод методов про калибровочную инвариантность (????)

Поэтому можно воспользоваться теоремой Нетер, чтобы найти сохраняющиеся величины при движении.

$$\Psi_u(\boldsymbol{r},t) = e^{-\mathrm{i}u}\Psi(\boldsymbol{r},t), \quad \Psi_u^\dagger(\boldsymbol{r},t) = e^{\mathrm{i}u}\Psi^\dagger(\boldsymbol{r},t)$$

$$\frac{dS}{du} = \int dt d^3r \partial_\mu \left\{ \frac{\partial \mathcal{L}}{\partial \partial_\mu \Psi}\frac{\partial \Psi_u}{\partial u} + \frac{\partial \mathcal{L}}{\partial \partial_\mu \Psi^\dagger}\frac{\partial \Psi_u^\dagger}{\partial u} \right\} = 0$$

(???)

В итоге у нас равен нулю 4-дивергенция тока:

$$\partial_\mu \mathcal{J}^\mu = 0, \quad \mathcal{J}^\mu = \frac{\partial \mathcal{L}}{\partial \partial_\mu \Psi}\frac{\partial \Psi_u}{\partial u} + \frac{\partial \mathcal{L}}{\partial \partial_\mu \Psi^\dagger}\frac{\partial \Psi_u^\dagger}{\partial u}$$

$$\int dt d^3r \partial_0 \mathcal{J}^0 + \int dt d^3r \boldsymbol{\nabla}\cdot\mathcal{J} = \int d^3r \mathcal{J}_0 \Big|_{t_1}^{t_2} + \int dt \oint d^2s \cdot \mathcal{J} = 0$$

$$Q = \int d^3r \mathcal{J}_0$$

$$\frac{\partial \Psi_u}{\partial u} = -\mathrm{i}\Psi, \quad \frac{\partial \Psi_u^\dagger}{\partial u} = \mathrm{i}\Psi^\dagger$$

$$\mathcal{L} = \mathrm{i}\hbar\Psi^\dagger\dot{\Psi} - \tfrac{\hbar^2}{2m}\left(\nabla\Psi^\dagger\right)\cdot(\nabla\Psi)$$
$$\mathcal{J}_0 = c\hbar\Psi^\dagger\Psi, \quad \mathcal{J} = -\tfrac{\mathrm{i}\hbar^2}{2m}\left[\Psi^\dagger\nabla\Psi - \left(\nabla\Psi^\dagger\right)\Psi\right]$$

$$\mathcal{J}^\mu = \hbar(c\rho, j)$$

$$\hat{p}_\mu\Psi = \mathrm{i}\hbar\partial_\mu\Psi = \mathrm{i}\hbar\left(\frac{\partial\Psi}{c\partial t}, \boldsymbol{\nabla}\Psi\right), \quad p_\mu = (E/c, -\boldsymbol{p})$$

(пропущено много)

в итоге лагранжиан является калибровочно инвариантным относительно локальных преобразований.

$$\mathcal{L} = c\Psi^\dagger\left(\hat{p}_0 + \frac{e}{c}A_0\right)\Psi + \frac{1}{2m}\left(\hat{p}\Psi + \frac{e}{c}\boldsymbol{A}\Psi\right)^\dagger\cdot\left(\hat{p}\Psi + \frac{e}{c}\boldsymbol{A}\Psi\right)$$

как будто в итоге у нас обычная механика...

27.1.2 Ways to Combine Quantum Mechanics and Gravity

(мб этому разделу тут не место, но идея в том, что вообще-то можно было бы иначе все строить, тогда бы гравитация добавилась. в любом случае, подробно - или под конец записи или в других записях.)

27.1.3 On the Construction of Quantum Mechanics Without Imaginary Numbers (???)

(то пока не знаю, вроде нельзя, почему - пока не готов объяснить.)

27.1.4 Quantum Mechanics Methods in Solid-State Physics

(тут компактно их укажу, особо большой главы не нужно, достаточно просто указать)

Об описании взаимодействия частиц

(левитов Шитов глава 4, пока я не настолько освоился с основами, чтобы этим заниматься. потом напишу суть.)

27.2 How to Understand Quantum Mechanics?

(по идее все про это тут)

27.2.1 Copenhagen Interpretation

Многие физики по поводу смысла квантовой механики не задумываются, а чуть что - понимают то, что называется копенгагенской интерпретацией. Действительно, это простая и удобная конструкция, понимание которой необходимо для понимание квантовой механики. Обсудим ее, понимая, что есть также другие интерпретации, которые обсуждаются в другом разделе.

обзор

Копенгагенская интерпретация — интерпретация (толкование) квантовой механики, которую сформулировали Нильс Бор и Вернер Гейзенберг во время совместной работы в Копенгагене около 1927 года[1][2][3][4]. Бор и Гейзенберг усовершенствовали вероятностную интерпретацию волновой функции, данную М. Борном, и попытались ответить на ряд вопросов, возникающих вследствие свойственного квантовой механике корпускулярно-волнового дуализма, в частности на вопрос об измерении.

Основные идеи копенгагенской интерпретации

Физический мир состоит из квантовых (малых) объектов и классических измерительных приборов.

Уравнение Шрёдингера (волновой функцией) описывает изменение квантового состояния объектов.

Изменение состояния классических измерительных приборов описывается необратимым статистическим процессом измерения характеристик квантовых микрообъектов.

В процессе взаимодействия микрообъекта с атомами измерительного прибора происходит редукция волновой функции измеряемого микрообъекта, то есть сведение суперпозиции к одному состоянию. Этот результат не следует из уравнения Шрёдингера.

Согласно копенгагенской интерпретации, квантовая механика описывает не микрообъекты сами по себе, а их свойства, проявляющиеся в макроусловиях, создающихся классическими измерительными приборами в процессе акта наблюдения.

Поведение атомных объектов невозможно резко отграничить от их взаимодействия с измерительными приборами, фиксирующими условия, при которых происходят

явления[5] Квантовая механика является статистической теорией, вследствие того, что измерение начальных условий микрообъекта изменяет его состояние и приводит к вероятностному описанию исходного положения микрообъекта, которое описывается волновой функцией[6]. Центральным понятием квантовой механики является комплексная волновая функция. Можно описать изменение волновой функции до нового измерения. Его ожидаемый результат зависит вероятностным образом от волновой функции. Физически значимым является лишь квадрат модуля волновой функции, означающий вероятность нахождения изучаемого микрообъекта в некотором месте пространства.[7][8]

Закон причинности в квантовой механике выполняется по отношению к волновой функции, изменение которой во времени полностью определяется её начальными условиями, а не по отношению к координатам и скоростям частиц, как в классической механике. Вследствие того, что физический смысл имеет лишь квадрат модуля волновой функции, начальные значения волновой функции невозможно полностью найти в принципе, что приводит к неопределённости знаний о начальном состоянии квантовой системы.[9]

Философскую основу копенгагенской интерпретации составляют гносеологические принцип наблюдаемости (исключение, насколько возможно, из физической теории утверждений, которые не могут быть проверены непосредственным наблюдением)[10], принцип дополнительности (волновое и корпускулярное описание микрообъектов являются дополнительными друг к другу)[11], принцип неопределённости (координата и импульс микрообъектов не могут быть определены независимо друг от друга и с абсолютной точностью)[11], принцип статистического детерминизма (данное состояние замкнутой физической системы определяет её последующее состояние не однозначно, а лишь с определённой вероятностью, описывающей меру возможности осуществления заложенных в прошлом тенденций изменения) и принцип соответствия (законы квантовой механики переходят в законы классической, когда можно пренебречь величиной кванта действия).

в квантовой физике данные об атомных объектах, полученные при помощи разных экспериментальных установок, находятся в своеобразном дополнительном отношении друг к другу.[12] соотношения неопределённостей Гейзенбергадают связь (обратную пропорциональность) между неточностями допустимого в квантовой механике фиксирования тех кинематических и динамических переменных, которыми в классической механике определяется состояние физической системы.[12] Серьёзным преимуществом копенгагенской интерпретации является то, что она не использует детальных высказываний о непосредственно физически не наблюдаемых величинах и при минимуме используемых предпосылок выстраивает систему понятий, которые исчерпывающим образом описывают имеющиеся на сегодня экспериментальные факты[13].

Смысл волновой функции

Копенгагенская интерпретация предполагает, что на волновую функцию могут влиять два процесса:

унитарная эволюция согласно уравнению Шрёдингера процесс измерения По поводу первого процесса не возникает разногласий ни у кого, а по поводу второго имеется ряд различных интерпретаций, даже в пределах самой копенгагенской интерпретации. С одной стороны, можно полагать, что волновая функция является реальным физическим объектом и что она во время второго процесса претерпевает коллапс, с другой стороны, можно считать, что волновая функция — лишь вспомогательный математический инструмент (а не реальная сущность), единственное предназначение которой — это

давать нам возможность рассчитывать вероятности. Бор подчёркивал, что единственное, что можно предсказывать — это результаты физических опытов, поэтому дополнительные вопросы относятся не к науке, а к философии. Бор разделял философскую концепцию позитивизма, которая требует, чтобы наука говорила только о реально измеримых вещах.

В классическом двухщелевом опыте свет проходит через две щели и падает на экран, где появляются тёмные и светлые интерференционные полосы. Это можно объяснить тем, что в некоторых местах световые волны взаимно усиливаются, а в других — гасятся. С другой стороны, эксперимент показывает, что свет обладает и свойствами потока частиц, а такие объекты, как электроны могут проявлять и волновые свойства и тоже могут давать интерференционную картину.

Это ставит несколько интересных вопросов. Допустим, двухщелевой эксперимент проводится с настолько низкой интенсивностью потока фотонов (или электронов), что каждый раз через щели проходит только по одной частице. Однако, когда экспериментатор сложит точки попадания всех фотонов на экран, он получит ту же интерференционную картину от накладывающихся волн, несмотря на то, что вроде бы опыт касался отдельных частиц. Это можно интерпретировать так, что мы живём в «вероятностной» вселенной — такой, что в ней с каждым будущим событием связана определённая степень возможности, а не в такой, что в каждый следующий момент может случиться всё что угодно.

Следствия копенгагенской интерпретации

Данный опыт ставит следующие вопросы:

Законы квантовой механики говорят о том, где частицы попадут в экран статистически и дают возможность рассчитать местоположение светлых полос, куда скорее всего попадёт много частиц и местоположение тёмных полос, куда скорее всего попадёт мало частиц. Однако для отдельной частицы законы квантовой механики не способны предсказать, где она окажется фактически. Каковы в таком случае правила поведения отдельных частиц? Что происходит с частицей между моментом испускания и моментом регистрации? Создаётся впечатление, что частица претерпевает взаимодействие с обеими щелями. И это кажется противоречащим тому, как может себя вести точечная частица. Тем более что, когда частица регистрируется, она оказывается точечной. Что заставляет частицу переключаться от статистического к нестатистическому поведению и обратно? Когда частица летит сквозь щели, её поведение описывается нелокализованной волновой функцией, которая одновременно проходит через обе щели. Когда же частица регистрируется, никогда не получается размытый волновой пакет, но всегда фиксируется точечная частица. Копенгагенская интерпретация отвечает на эти вопросы так:

Вероятностный характер предсказаний квантовой механики принципиально неустраним, то есть он вовсе не говорит о том, что наши знания ограничены, что мы не знаем значений каких-то скрытых переменных. В классической физике вероятность использовалась для описания результатов типа подбрасывания игральной кости, хотя фактически этот процесс считался детерминированным. То есть вероятности использовались вместо неполного знания. Напротив, копенгагенская интерпретация утверждает, что в квантовой механике результат измерения принципиально недетерминирован. Физика — это наука о результатах измерительных процессов. Измышления на тему того, что происходит за ними, неправомерны. Копенгагенская интерпретация отбрасывает вопросы типа «где была частица до того, как я зарегистрировал её местоположение» как бессмысленные. Акт измерения вызывает мгновенное схлопывание, «коллапс волновой функции». Это означает, что процесс

измерения случайно выбирает в точности одну из возможностей, допустимых волновой функцией данного состояния, а волновая функция мгновенно изменяется, чтобы отразить этот выбор. Оригинальная формулировка копенгагенской интерпретации породила ряд вариаций; наиболее уважаемая основана на подходе непротиворечивых событий («Копенгаген прав?») и понятии квантовой декогеренции, которая позволяет рассчитывать нечёткую границу между «микро» и «макро» мирами. Другие вариации различаются степенью «реалистичности» волнового мира.

Критика и недостатки копенгагенской интерпретации

Полнота квантовой механики (тезис 1) была подвергнута сомнению в мысленном эксперименте Эйнштейна, Подольского и Розена (ЭПР-парадокс), который был предназначен для того, чтобы доказать, что скрытые параметры должны существовать, чтобы теория не приводила к нелокальному и мгновенному «дальнодействию». Однако проверка ЭПР-парадокса на опыте при помощи неравенств Белла показала, что квантовая механика верна и что различные теории локальных скрытых параметров не согласуются с экспериментом.

Из всех трёх тезисов с физической точки зрения наиболее проблематичен последний, поскольку он ставит процессы измерения в особое положение, но не определяет ясно, что они такое, и не указывает на их отличительные черты.

Многие физики и философы не соглашаются с копенгагенской интерпретацией, как потому, что она не детерминистична, так и потому, что она вводит неопределённое понятие измерения, которое превращает вероятностные функции в достоверные результаты измерений.

Эйнштейн был убежден в неполноте описания физической реальности, даваемого квантовой механикой в её копенгагенской интерпретации: «Думать так логически допустимо, но это настолько противоречит моему научному инстинкту, что я не могу отказаться от поисков более полной концепции».[14]

Иллюстрируя это, Эйнштейн писал[прим. 1] Борну: «Я убеждён, что Бог не бросает кости», — а также восклицал в беседе с Абрахамом Пайсом: «Вы и вправду думаете, что Луна существует, лишь когда вы на неё смотрите?». Н. Бор отвечал ему: «Эйнштейн, не указывайте Богу, что делать». Эрвин Шрёдингер придумал знаменитый мысленный эксперимент про кота Шрёдингера, которым он хотел показать неполноту квантовой механики при переходе от субатомных систем к макроскопическим.

Аналогично вызывает проблемы необходимый «мгновенный» коллапс волновой функции во всём пространстве. Теория относительности Эйнштейна говорит, что мгновенность, одновременность, имеет смысл только для наблюдателей, находящихся в одной системе отсчёта — не существует единого для всех времени, поэтому мгновенный коллапс тоже остаётся не определён.

27.2.2 Other Attempts to Construct Quantum Mechanics

О квантовой механики без комплексных чисел (!??!?!)

(интересно, почему без них никуда, или все-таки есть ли способ без них???? хз вообще.)

27.3 Paradoxes

(по идее тут подробно все их соберу)

27.3.1 EPR

Связь ЭПР и космологии

Он нужен в космологии хотя бы где-то???

(а я хз на самом деле, мб где-то и встретил я его, раз написал. потом подумаю.)

Теория парадокса ЭПР

Согласно соотношению неопределённостей Гейзенберга, нет возможности одновременно точно измерить координату частицы и её импульс.

Предполагая, что причиной неопределённости является то, что измерение одной величины вносит принципиально неустранимые возмущения в состояние и производит искажение значения другой величины, можно предложить гипотетический способ, которым соотношение неопределённостей можно обойти.

Допустим, две одинаковые частицы A и B образовались в результате распада третьей частицы C.

В этом случае, по закону сохранения импульса, их суммарный импульс p A + p B должен быть равен исходному импульсу третьей частицы p C p C, то есть, импульсы двух частиц должны быть связаны.

Это даёт возможность измерить импульс одной частицы)A A) и по закону сохранения импульса p A p B = p C - p A рассчитать импульс второй)B B), не внося в её движение никаких возмущений.

Теперь, измерив координату второй частицы, можно получить для этой частицы значения двух неизмеримых одновременно величин, что по законам квантовой механики невозможно.

Исходя из этого, можно было бы заключить, что соотношение неопределённостей не является абсолютным, а законы квантовой механики являются неполными и должны быть в будущем уточнены.

Если же законы квантовой механики в данном случае не нарушаются, то измерение импульса одной частицы равносильно измерению импульса второй частицы.

Однако это создаёт впечатление мгновенного воздействия первой частицы на вторую в противоречии с принципом причинности.

27.4 Deeper Understanding of Philosophy of Quantum Mechanics

Подробно обсудим философию квантовой механики.

(сперва делаю важное, потом в свободное время Иванова М.Г. мб почитаю, пропишу этот раздел подробно. мб эзотерику обсужу также.)

(I'll merge it with the part 2 later)

27.4.1 Is QM Created This Way By The Way How Humans Want or By Nature?

(this question which Kant answered: by Humans, because all what we see is that we already analyze. so, all concepts are what we want to see, all "quantums" is our ideas, because this is what we understand. the discussion of this will be here)

27.4.2 Other Philosophical Questions

(unstructured, no time for it now, I'll do it later and put some of them to the first part)

интуитивное представление квантовой физики (????)

это естественно и очевидно, что в микромире все начнет делиться на части.

как уровни.

????

и что переходы должны не зависеть ни от чего, но если и зависеть - то только от природы, а значит, как раз это и происходит, вероятностное описание, вот мы и осознали, почему так.

что такое квант материи

обсудим это, и что мы описываем квантами?

принцип дополнительности

хз к чему он, просто выгрузка пока

мы с ним уже встречались, когда рассматривали атомы, тут хотелось бы сделать какие-то общие выводы про то, как работает мир.

сперва этот принцип во всей красе:

Перейти к поиску Принцип дополнительности — один из важнейших методологических и эвристических принципов науки, а также один из важнейших принципов квантовой механики, сформулированный в 1927 году Нильсом Бором.

Согласно этому принципу, для полного описания квантовомеханических явлений необходимо применять два взаимоисключающих («дополнительных») набора классических понятий, совокупность которых даёт исчерпывающую информацию об этих явлениях как о целостных.

Например, дополнительными в квантовой механике являются пространственно-временная и энергетически-импульсная картины.

Описания любого физического объекта как частицы и как волны дополняют друг друга, одно без другого лишено смысла, корпускулярный и волновой аспекты описания обязательно должны входить в описание физической реальности[1].

При получении информации об одних физических величинах, описывающих микрообъект, неизбежно теряется информация о других физических величинах, дополнительных к первым.[2]

о существовании эффекта наблюдателя

(? пока не разобрался, существует он, или нет?)

насколько правда то, что если наблюдаем за системой, она ведет себя иначе, чем без наблюдения?

пока что думаю, что это неправда и такого не бывает

В квантовой механике, «наблюдение» является синонимом измерения, «наблюдатель» — синонимом измерительной аппаратуры, а наблюдаемое — с тем, что можно измерить.

Одним из основных понятий квантовой механики является сформулированная ещё в 1924 году в совместной работе Бора, Крамерса и Слэйтера, интерпретация волновой функции ψ как волны вероятности, а не реальной волны, как предполагал де Бройль.

До измерения квантовая система находится в суперпозиции допустимых состояний.

Считается, что после измерения, которое определяет часть параметров системы, волновая функция скачком меняется, принимая вид, соответствующий измеренным значениям параметров[6].

Примером может служить кот Шрёдингера.

Наблюдение невозможно без взаимодействия наблюдаемого объекта с окружающей средой — чтобы наблюдатель мог определить параметры объекта, он должен получить информацию от такого взаимодействия.

Квантовый объект при этом неизбежно изменяет своё состояние.

Для элементарных частиц это очевидно, поскольку наблюдать такие частицы мы можем только по их взаимодействию (либо с фотонами, либо с веществом, через которое пролетает частица)[8].

В экспериментах с крупными молекулами, наблюдать которые можно по их тепловому излучению, было определено, что «эффект наблюдателя» проявляется и в отсутствие непосредственного воздействия наблюдателя на квантовый объект, но при любом взаимодействии (обмене энергией) между квантовой системой и окружающим пространством.

Экспериментаторы улавливали тепло (инфракрасные фотоны), излучённое нагретыми молекулами фуллерена C70, и чем выше была температура молекул, тем более классически вели себя нагретые молекулы.

В этих экспериментах было продемонстрировано, что величина квантовых эффектов обратна интенсивности взаимодействия квантового объекта с окружающей его средой, наличие наблюдателя при этом не имеет значения[9][8].

Таким образом, эффект наблюдателя меняет состояние квантовой системы, отражённое в главном её описании — волновой функции.

Более поздние исследования показали, что такое влияние наблюдателя распространяется не только на изучаемую частицу, но и на взаимодействовавшую с ней, приведя к понятию «запутанных состояний».

Волновая функция связанной частицы также испытывает скачок своего состояния после наблюдения, что используется в квантовой криптографии.

Поскольку прослушивание канала передачи данных является наблюдением, этот эффект можно отследить

(????)

Доказала ли квантовая механика, что реальности не существует?

(там вроде про это рассуждения есть, посмотрю потом. чисто тема для научпоп видео или разговоров.)

27.4.3 Criticism by Fock of Bohr's Views on Quantum Mechanics (!?!??!)

Criticism by Fock of Bohr's Views on Quantum Mechanics (!?!??!)

В 1948 г. на страницах издаваемого в Швейцарии журнала «Диалектика» состоялась дискуссия по принципиальным вопросам квантовой механики. В этой дискуссии приняли участие многие выдающиеся зарубежные физики: Бор, Гейзенберг, Эйнштейн, Паули и другие, статьи которых были напечатаны в № 7; 8 упомянутого журнала за 1948 г. Руководящей является статья Бора «О понятиях причинности и дополнительности». Эту статью можно рассматривать не только как выражение взглядов собственно копенгагенской школы, но и как выражение тех взглядов на квантовую механику, которые господствуют среди зарубежных физиков. Взгляды эти вырабатывались на основе идеалистической философии— так называемого позитивизма, нзсовместимой с марксистсколенинской философией диалектического материализма. Неправильные философские установки, применённые к какой-либо конкретной области науки, почти неизбежно приводят к ошибкам в самой этой области. Поэтому особенно важно

проанализировать, нет ли во взглядах представителей копенгагенской школы на квантовую механику помимо неприемлемых общефилософских высказываний, неправильность которых для советского читателя очевидна, также и конкретных ошибок, приводящих к неправильному толкованию самой квантовой механики. Поскольку упомянутая статья Бора представляет резюме этих взглядов, формулированное признанным главой копенгагенской школы, она даёт удобный материал для такого анализа. Чтобы быть точными, нам придётся подробно изложить содержание упомянутой статьи Бора и привести из неё достаточно полные цитаты. Во вводной части своей статьи Бор говорит о причинном способе описания явлений в классической физике, и пишет: «теория относительности, которая придала классической физике небывалое единство и широту, позволила точно формулировать принцип причинности в самом общем виде». По этому поводу можно заметить следующее. Несомненно, что в области физики теория относительности значительно уточнила понятие причинности. Точная же формулировка принципа причинности в самом общем виде есть вопрос общефилософский и решение этог о вопроса принадлежит классикам марксизма. Дальше Бор пишет следующее: «Совершенно новое положение вещей в физической науке создалось, однако, благодаря открытию универсального кванта действия. Это открытие обнаружило первичную черту неделимости атомных процессов, идущей гораздо дальше старого учения об ограниченной делимости материи, которое было первоначально введено для причинного объяснения свойств вещества и служило основанием этому объяснению. Эта новая черта не только совершенно чужда классическим теориям механики и электромагнетизма, но даже несовместна с самой идеей причинности». Таким образом. Бор утверждает, что существование кванта действия несовместно с самой идеей причинности. Чем он это мотивирует? Продолжаем цитату. «В самом деле, если задано состояние физической системы, то этим, очевидно, ещё не определяется, какой именно из различных элементарных процессов перехода в другие состояния будет иметь место. При учёте квантовых эффектов приходится существенным образом оперировать с понятием вероятности различных возможных процессов перехода». , Сказанное здесь верно, но никак не может служить доводом в пользу несоблюдения принципа причинности. Прежде всего, причинность не сводится к однозначной детерминированности, а включает более общее понятие о закономерности. Кроме того, в квантовых явлениях необходимо различать между развитием во рремени состояния системы, находящейся в строго определённых физических условиях, и тем скачкообразным изменением состояния, которое приходится вводить при резком и не поддающемся точному контролю изменении физических условий. (Такое резкое изменение физических условий бывает необходимо для измерения той или иной физической величины).Совершенно естественно, что в квантовой механике волновое уравнение, описывающее с той или иной степенью точности состояние системы, находящейся в определённых физических условиях, перестаёт быть применимым, когда эти условия резко меняются и становятся не вполне определёнными. Когда физические условия заданы, изменение состояния происходит но определённому закону, в полном соответствии с принципом причинности. Когда же эти условия резко и неощщделённым образом меняются, никак нельзя требовать, чтобы изменение состояния было предопределено наперёд. Но и это изменение состояния отнюдь не является бессистемным, а подчиняется определённым вероятностным законам, что также соответствует принципу причинности. Состояние объекта в момент времени, непосредственно предшествующий внешнему вмешательству, определяет собой вероятность того или иного поведения объекта при этом вмешательстве. Можно даже сказать, что и само состояние характеризуется вероятностью того или иного поведения объекта при всевозможных потенциальных внешних воздействиях. К этому вопросу мы

вернёмся в дальнейшем. Далее Бор указывает на наличие корпускулярных и волновых свойств частиц и говорит, что «всякое определение постоянной Планка основано на сопоставлении двух аспектов явления, которым соответствуют картины, не совместимые в рамках классических теорий». Последнее замечание представляется нам довольно тривиальным, так как из опытов, в которых не проявляются квантовые эффекты, конечно, нельзя определить постоянной Планка. Бор, однако, после этого говорит: «При таком положении вещей мы встречаемся с необходимостью радикального пересмотра самых основ для описания и объяснения физических явлений», предпосылая эти слова изложению основных идей квантовой механики в его понимании. Переходя к изложению квантовой механики. Бор прежде всего подчёркивает, «что описание экспериментальной установки и регистрация наблюдений всегда должны быть выражены на обычном языке, пользующемся терминологией классической физики». Само по себе это утверждение бесспорно верно. Однако из него отнюдь нельзя делать таких выводов, какие делает Бор, а именно, что всё остальное, кроме описания экспериментальной установки и регистрации наблюдений, имеет лишь символический характер. К этой точке зрения Бора мы вернёмся ниже. Затем Бор говорит: «Тот факт, что квантовые явления не могут быть анализированы в духе классической физики, влечёт за собой невозможность разделить поведение атомных объектов от их взаимодействия с измерительными приборами, которые фиксируют условия, в каких происходят явления. В частности, неделимость типичных квантовых эффектов выражается в том,что всякая попытка подразделить явление требует изменения экспериментальной установки, каковое изменение вносит новые источники неконтролируемого взаимодействия между объектами и измерительными приборами». В первой фразе правильно указывается на то, что состояние атомных объектов и их «поведение», т. е. изменение состояния, зависят от внешних условий, и что поэтому существенно необходимо эти внешние условия фиксировать. Мысль, высказанная во второй фразе, также в общем правильна, хотя слова о неконтролируемом взаимодействии, строго говоря, лишены точного смысла. В самом деле, здесь речь идёт о взаимодействии в самом акте измерения. Но что значит «контролировать»? По существу, это значит «измерять». Таким образом, «неконтролируемость» означает, по нашему мнению, просто невозможность вставить добавочное измерение, не нарушая условия данного измерения. Повидимому, слова Бора о неконтролируемом взаимодействии представляют попытку пояснить на языке классической физики то положение вещей, которое возникает из соотношений Гейзенберга, применённых к взаимодействию между объектом и прибором. Что бы ни понимал под этими словами Бор, с нашей точки зрения они во всяком случае никакого более глубокого смысла не имеют и тем более не должны пониматься в смысле какого-либо утверждения о непознаваемости процесса взаимодействия и т. п. Утверждение Бора о невозможности разделить поведение атомных объектов от их взаимодействия с измерительными приборами также можно принять лишь с оговорками. Как видно из дальнейшего, Бор понимает эго утверждение не в смысле взаимосвязи между изучаемым объектом и окружающим его полем и внешними предметами, в частности измерительными приборами, а в том смысле, что атомный объект как бы растворяется в измерительном приборе и становится менее реальным, чем измерительный прибор. Кроме того. Бор не указывает, что именно он разумеет под измерительным прибором: считает ли он, что измерительный прибор включает ту часть, где объект находится в фиксированных внешних условиях и явление развивается без помех, или же он разумеет под прибором то устройство, которое вводится в действие лишь в последней стадии опыта и служит для регистрации результата измерения. Например, в явлении диффракции электронов мы имеем фиксированные внешние условия внутри кристаллической решётки, сквозь которую проходит электрон

(регулярное расположение атомов, упругий характер столкновении электронов с ними). Для наблюдения диффракционной картины мы можем поставить позади кристалла фотографическую пластинку, ряд счётчиков иль какой-нибудь иной прибор, способный измерять координату электрона. Детали его устройства безразличны; в случае фотопластинки или счётчика мы имеем дело с усилительным устройством, в котором развиваются процессы лавинного характера. Наличие же кристалла для явления диффракции существенно: если крлсгалла нет, то и диффракции не будет, а если он есть, то диффракция будет, независимо от того, как будет регистрироваться диффракционная картина и будет ли она вообще регистрироваться. Для краткости мы будем называть ту часть прибора, где происходит само явление, рабочей частью прибора, а ту часть, где оно регистрируется,— регистрирующей частью. В нашем примере рабочей частью является кристалл, а регистрирующей — фотопластинка или счётчик.

Кроме рабочей и регистрирующей частей можно говорить о приготовляющей части: это—та часть, которая фиксирует состояние объекта перед его попаданием в рабочую часть. В налам примере приготовляющей частью является источник монохроматического пучка электронов, а также диафрагмы и другие устройства, поставленные перед кристаллом. Необходимо отметить, что, поскольку явление может происходить и в естественных условиях, приготовляющая, а также рабочая часть могут осуществляться сами собою и лишь регистрирующая часть требует, вообще говоря, особого устройства. Упомянутая выше неточность Бора заключается в том, что он не проводит разграничения между различными частями измерительного прибора и оставляет открытым, разумеет ли он под измерительным прибором только его регистрирующую часть или же он включает в это понятие также и рабочую часть. Слова о «неконтролируемом взаимодействии» относятся, очевидно, к регистрирующей части, тогда как утверждение, что измерительные приборы фиксируют условия, в каких происходят явления, повидимому, может относиться только к рабочей части.:. ' В результате этой неточности (возможно умышленной") затушёвано существенно важное различие между поведением объекта в фиксированных внешних условиях и его поведением в условиях, не вполне определённых. Поведение объекта в фиксированных внешних условиях вполне определяется начальным состоянием и свойствами самого объекта и может быть весьма точнэ оплсано на язык квантовой механики. Результат же последнего эгапа измерения, связанного с взаимодействием объекта с регисгрируюдей частью измерительного прибора, должен уже оплсызагься Hi языке классической физики, причём вероятность того или иного результата вычисляется по формулам квантовой механики. Из сказанного им Бор делает следующий вызэд: «При таком положенлл вещей прлллсызлнлг атомным объектам обычных, условно прлнлгых, флзлческих атрибутов (conventional physical attributes) связано с неоднозначностью». Несколько туманная фраза об услозных флзлческих атрибутах требует расшифровки. Еслл здесь разумеется невозможность приписывать, например, электрону при всех услозиях определённую координату или определённое количество движения, то с этим можно согласиться, поскольку, согласно квантовой механике, какие бы то ни было классические модели атомных объектов имеют лишь ограниченную применимость*). Но фраза сосгазланд в такой общей форме, что под физическими атрибутами могут разуметься '*) Толкование соотношений неопределённости Гейзенберга как принципа ограниченной применимости кпссшескях мэдглея дало в нашей работе (Вестник Ленинградского университета, № 4, стр. 31, 191Э).

и такие свойства электрона, как заряд, масса, спин, свойства, связанные с видом оператора энергии и определяющие взаимодействие электрона с другими частицами и с внешними полями. Все эти свойства совершенно объективны и несомненны, и ни о какой их условности не может быть и речи. Поэтому, если Бор имел здесь в виду оспаривать

наличие у атомных объектов объективных свойств, подобных перечисленным, то в этом с ним никак согласиться нельзя. Дальше Бор вводит свой термин «дополнительность» (сперва в применении к наблюдениям, произведённым при различных экспериментальных установках) и переходит к характеристике квантовой механики. Чрезвычайно любопытна та роль, которую отводит Бор квантовой механике в описании и объяснении атомных явлений. Вместо того, чтобы прямо признать, что предметом и назначением квантовой механики является более глубокое изучение свойств атомных объектов. Бор с самого начала говорит: «Надлежащим средством для дополнительного способа описания является аппарат квантовой механики». Тем самым роль квантовой механики заранее сводится к составлению формальных рецептов для вычисления вероятностей различных результатов наблюдений, без всякого проникновения в сущность явления. Характеризуя аппарат квантовой механики. Бор всячески подчёркивает его будто бы исключительно символический характер. Бор говорит, что в этом аппарате «сохраняются канонические уравнения классической механики, но физические переменные заменяются символическими операторами, подчинёнными некоммутативной алгебре». Непонятно, почему математический аппарат квантовой механики более символичен, чем аппарат любой другой физической теории. Математика всегда оперирует с символами, но поскольку в физической теории эти символы допускают определённое физическое толкование, они перестают быть абстрактными символами, а отражают действительность. Так обстоит дело независимо от сложности применяемого математического аппарата. Уравнение Шредингера квантовой механики не более и не менее символично, чем уравнение Гамильтона— Якоби классической механики. Бор же подчёркивает, что классическая механика имеет дело с физическими переменными, тогда как квантовая механика — будто бы лишь с символическими операторами. Трудно удержаться от мысли, что такое противопоставление нужно Бору для того, чтобы оставить за собою право подвергнуть сомнению реальность существования и свойств атомных объектов, с которыми оперирует квантовая механика. Стремление устранить прямое физическое толкование аппарата квантовой механики, оставив за ним только символический смысл, доводит Бора до абсурда. Так, он говорит: «Самые же эти символы не допускают наглядной интерпретации, на что указывает уже употребление мнимых чисел».

Как будто бы мнимые числа заключают в себе что-то мистическое и употребление и исключает возможность наглядной интерпретации! Ведь с ним; постоянно оперирует и классическая физика, особенно электро техника. Свою мысль о том, что математический аппарат квантово механики будто бы не связан непосредственно со свойствами атом ных объектов (о реальности которых Бор вообще нигде не упоминает), а играет чисто вспомогательную роль для координаций результатов измерений. Бор выражает и прямо. Он пишет: «Весь аппарат следует рассматривать как средство для вывод, предсказаний, однозначного или статистического характера, относя щихся к результатам, которые могут быть получены при опре делённых экспериментальных условиях». Эта мысль, что не просто знание объективных свойств реаль ных атомных объектов, а нечто чисто символическое являете! основой для предсказаний, несомненно внушена Бору его идеали стической философской установкой. Бор не является вполне по следовательным идеалистом, поскольку он, повидимому, всё же признаёт реальность тех явлений, которые могут быть описань на языке классической физики, но его точка зрения на квантовук механику является бесспорно идеалистической. Переходя затем к рассмотрению соотношений Гейзенберга, Бор указывает на «взаимно исключающие условия, при которых можно без противоречий пользоваться локализацией в пространстве и времени, с одной стороны, и законами сохранения механики, с другой». «В самом деле, — говорит Бор,—всякая попытка локализации атомного объекта в

пространстве и времени требует такого экспериментального устройства, в котором происходит прин шпиально не поддающийся контролю обмен количеством движения и энергией между объектом и масштабами и часами, определяющими систему отсчёта. Обратно, никакое устройство, пригодное для контроля над балансом количества движения и энергии, не допускает точного описания явлений, как цепи событий, локализованных в пространстве и времени». Всё это совершенно верно при условии, что анализ поведения атомного объекта производится на основе классической механики (о чём сам Бор и говорит в следующей своей фразе). Но на самом целе лишь последний этап измерения (связанный обычно с действием какого-нибудь усилительного устройства) требует такого классического анализа. Предшествующее же поведение объекта, когда он находился ещё в фиксированных внешних условиях, может быть гораздо более точно проанализировано на основе квантовомеханических представлений. Поэтому нельзя согласиться с утверждением Бора, что «соотношения неопределённости явным образом указывают на ограниченость причинного расмотрения». Соотношения неопределённости налагают ограничения на применимость классических моделей, но принцип причинности не составляет монополии классической физики, и отказ от классических моделей не означает отказа от причинности. Переходя к перечислению положительных до стижений квантовой механики, Бор как бы забывает о том, что он на предыдущих страницах придавал её математическому аппарату лишь чисто символическое значение и связывал его не со свойствами атомных объектов, а с координадией результатов измерений. Бор пишет следующее: «Квантовая механика представляет обобщение классической механики, позволяющее учитывать существование кванта действия. Рамки её достаточно широки для того, чтобы включать в себя объяснение наблюдаемых на опыте закономерностей, не поддающихся описанию классическим способом. Укажем здесь на характерную устойчивость атомов, наличие которой дало первый толчок к развитию квантовой механики. Кроме того, можно указать на своеобразные закономерности, наблюдаемые в системах, составленных из одинаковых частиц, например фотонов или электронов. Эти закономерности играют решающую роль в равновесном излучении и в свойствах вещества. Как известно, они адекватно отображаются свойствами симметрии волновых функций, представляющих состояния сложных систем». В приведённой цитате Бор как бы переходит на материалистическую?иу зрения— на точку зрения учёного-естествоиспытателя. Он говорит об объективных свойствах атомов .(устойчивость), об объективно существующих закономерностях и об отображении их математическим аппаратом квантовой механики. С этими высказываниями можно вполне согласиться. В то же время нельзя не видеть их противоречия с тем, что Бор говорил несколькими страни ими выше. Но на этой магерчалисгической точке зрения Бор остаётся недолго. После разбора мысленного опыта, послужившего в своё время (1935 г.) предметом дискуссии между Бором и Эйнштейном, Бор возвращается к вопросу о предмете квантовой механики говорит, что в квантовомеханическом описании «мы имеем дело с математически непротиворечивой схемой, которая подходит в пределах своей области применимости) ко всякому измерительному процессу».

Таким образом, Бор здесь опять придаёт кванювой механике значение схемы, применяемой для координадии результатов измерительных процессов. Об отображении квантовой механикой объективных свойств реальных атомных объектов больше нет и речи. Особенно ярко идеалистическая философская установка Бора проявляется в рекомендуемом им толковании понятия «явление». Бор пишет: «Мы бы очень настаивали на том, чтобы. слово явление" употреблялось только в ограниченном смысле. Слово явление" должно относиться только к наблюдениям, произведённым в точно определённых условиях, включая указания о всём опыте в целом». Ввиду

важности этого определения для характеристики философской позиции Бора мы приведём соответствующую цитату, (на которую одобрительно ссылается Паули в своей редакционной статье) также и в подлиннике: «As a more appropriate way of expression, one may strongly advocate limitation of the use of the word phenomenon to refer exclusively to observations obtained under specified circumstances, including an account of the whole experiment» (Dialectica, 7/8, 1948, стр. 317). Проанализируем это определение. Во-первых, в нём отсутствует всякое указание на тот объект, который собственно и производит явление. Ссылка на объект заменена ссылкой на производимые наблюдения. Во-вторых, в нём не учтено, что собственно измерение составляет лишь последнюю стадию постановки опыта, а этой последней стадии должно предлзствоиать приготовление самого явления по возможности в чистом виде, т. е. в точно определённых условиях; последняя же стадия эти условии заведомо нарушает, о чём много раз в других местах говорит и сам Бэр, когда упоминает о «неконтролируемом взаимодействии». В последних словах определения Бора подчёркнуто, что опыт должен рассматриваться в целом, т. е. без подразделения на стадии; новидимому Бэр ставит это в связь с тем, что он говорил раньше о неделимости атомных процессов. Мзжду тем, если отказаться от подразделения опыта на стадии, то получится противоречие даже в самих словах Бора, который, с одной стороны, говорит о точно определённых условиях, а с другой стороны, неоднократно подчёркивает, что с измерением связано «неконтролируемое взаимодействие» между объектом и прибором. Ясно, что «точно определённые условия» и «неконтролируемое взаимодействие» могут относиться только к разным стадиям опыта. Необходимость подразделения опыта на невозмущённое явление и на самый акт измерения ясна сама по себе. Ведь невозмущённое явление может происходить и в естественных условиях, на которые мы даже не можгм повлиять (например, излучение атомов на какой-нибудь звезде). Таким образом, предлагаемое Бором определение не отвечает самым основным научным требованиям и является ошибочным как с точки зрения философии, так и с точки зрения физики. Философская ошибка Бора очевидна В угоду позитивистской идеалистической философии он стремится избежать даже упоминания об объекте, подлежащем изучению в данном опыте; это нужно ему для того, чтобы рассматривать этот объект только как вспомогательное логическое построение, необходимое для координации показаний приборов. Если Бор и не говорит этого прямо, то он расчищает путь к такому толкованию, и по этому пути идут затем другие, более открытые, приверженцы идеалистической философии. Но мы хотели бы здесь особенно подчеркнуть физическую ошибку Бора, которая, быть может, не столь очевидна, но не менее важна. Ведь именно путём неправильного толкования физических фактов зарубежные физики-идеалисты и пытаются обосновать свою философию. Основную физическую ошибку Бора, которая отражается не только на данном им определении «явления», но и на его понимании квантовой механики и которая проходит через всю егл статью, мы видим в следующем. Бор игнорирует, что в физическом эксперименте помимо начальной и конечной стадий (приготовления объекта и собственно акта измерения) существует ещё и средняя стадия, когда определённым образом приготовленный объект находится в фиксированных внешних условиях. Подразделение эксперимента на стадии не умозрительно, а зполне реально. Ему соответствует (в тех случаях, когда весь эксперимент проходит в лабораторных условиях) подразделение экспериментальной установки на приготовляющую, рабочую и регистрирующую части. Игнорируя среднюю стадию эксперимента, Зор как бы хочет отвлечь наше внимание от самой сущности тления, от той его части, которая может быть наиболее глубоко «учена методами квантовой механики. Ведь именно к этой средней стадии и применимо волновое уравнение квантовой механики, тогда как приготовление объекта и результат измерения должны

шисываться на языке классической физики. Состояние объекта з средней стадии описывается волновой функцией. Состояни е)то характеризуется, как мы уже говорили, вероятностью того или иного потенциального поведения объект а при каждом из возможны х внешни х в о з1ействий. Состояние даёт как бы настройку объекта, которая гвляется чем-то вполне реальным, несмотря на то, что для опре- (еления этой настройки нужно её нарушить. То обстоятельство, [то волновая функция характеризует поведение объекта не в слассическом смысле, не самого по себе, а лишь по отношению к конкретному внешнему воздействию, позволяет говорить о не абсолютном характере волновой функции в отличие от абсолютюго характера полей классической физики. Волнова я функция представляет новую (по сравнению с классической физикой) форму описани я состояни я объекта.

Игнорируя среднюю стадию эксперимента, Бор хочет свести его к приготовлению и измерению, которые описываются на языке классической физики с учётом лишь соотношения неопределённостей. Тем самым он принижает роль квантовой механики (оставляя за ней только некий символический смысл) и преувеличивает) значение соотношения неопределённостей. На самом дгле это соотношение ограничивает применимость классической механики(ничего не говорит о сущности квантовой механики. Существенная часть квантовой механики, позволяющая глубже проникнуть в изучение свойств атомных объектов, формулируется не при помощи соотношения неопределённостей, а при помощи математического аппарата, включающего в себя операторы в гильбертовом пространстве, волновые уравнения, волновые функции и т. и. Соотношение неопределённостей для координат и количества движения является следствие м аппарата квантовой механики, и лишь соотношение для энергии и времени, относящееся к акту измерения, вводится отдельно, причём и тут должно быть показано, что оно не противоречит уравнению Шредингера. Переоценка соотношения неопределённостей приводит Бора к далеко идущей переоценке его принципа дополнительности. Первоначально под дополнительностью разумелось то положение вещей, которое вытекало непосредственно из соотношения неопределённостей: дополнительность относилась к неопределённостям в координате и в количестве движения (в смысле их обратной пропорциональности) и термин «принцип дополнительности» понимался как синоним соотношений Гейзенберга*). Очень скоро, однако. Бор стал видеть в своем принципе дополнительности некий универсальный принцип, ограничивающий не только возможности описания в духе классической физики, но и возможности всякого научного описания, и применимый не только в физике, но и в биологии, психологии, социологии и во всех науках. Такая точка зрения проводится и в разбираемой статье Бора (на последних страницах). Ввиду явной необоснованности такой точки зрения мы её разбирать здесь не будем. Однако, поскольку термин «принцип дополнительности» потерял свой первоначальный смысл и стал употребляться как обозначение для несуществующих ограничений познания и для других неправильных понятий, лучше всего от него отказаться. В заключительных словах своей статьи Бор возвращается к своей мысли о том, что идея дополнительности призвана заменить *) В частности, в нашей статье в журнале «Под знаменем марксизма» № 1, за 1938 г., стр. 149, термин «принцип дополнительности» употребляется исключительно в смысле соотношений Гейзеноерга собою прежнюю идею причинности и что квантовая механика осуществляет эту замену в области физики. Нам кажется, однако, что квантовая механика доказывает как раз обратное. В ней найдены новые-форм ы выр а жен и я принцип а причинности, который наряду с другими принципами философии диалектического материализма останется надёжным руководителем в нашем стремлении к познанию природы.

27.4.4 Universe from the Point of View of Quantum Mechanics

о том, сколько времени помнит Вселенная то, что было в прошлом

есть одна точка зрения, что вселенная все помнит, и где-то да будут точно следы чего угодно из прошлого.

вторая точка зрения, что информация через некоторое время стирается, и все, прошлое абсолютно нигде не сохраняется.

что и насколько верно с точки зрения квантовой механики?

очень важный вопрос, а мне даже нечего сказать про него...

27.4.5 On the Applications of Quantum Mechanics Principles to Non-Quantum Objects

(????)

27.4.6 On the Limits of Applicability of Quantum Mechanics

(очень важный и большой вопрос, подробно отвечу на него)

27.4.7 On the Determinism of the World

(потом пообсуждаю, что там с ней. когда она есть, когда нет.)

об обратимости (?!!!)

27.4.8 On the Possibility of Predicting Future and Past (?)

(a really good question)

27.5 Some Hypothetical Projects

27.5.1 On Quantum Teleportation

(тут основное, что я про это знаю, подробнее - в статье напишу. морозов методичку писал, с нее начать можно)

А нельзя ли поставить процесс редукции волновой функции на службу?

Можно: был предложен защищенный от прослушивания квантовый канал связи.

Теория

Опишем принцип его работы на примере упрощенной схемы.

Пусть мы посылаем по нашему каналу последовательность нулей и единиц.

В случае посылки нуля создается пара фермионов со спином $1/2$ в состоянии

$$\Phi^{-}_{1,2} = \left(\frac{1}{\sqrt{2}}\right)(|\uparrow,\uparrow\rangle - |\downarrow,\downarrow\rangle)$$

а в случае посылки единицы в состоянии, описываемом выражением (5). Проекция спина фермиона 1 регистрируется и записывается отправителем сообщения A, а проекция спина фермиона 2 его получателем B.

Если кто-нибудь попытается перехватить сообщение на

пути к получателю, это приведет к редукции волновой функции второй частицы и будет замечено получателем.

Но по своим записям получатель не может ничего прочитать.

Ведь и в случае посылки нуля, и в случае посылки единицы получатель может зарегистрировать как проекцию спина $+1/2$, так и проекцию спина -1/2.

Одни измерения получателя не несут информации.

Чтобы понять послание он должен получить по обычному каналу связи (например, телефону) результаты измерений отправителя.

То есть информация передается не со сверхсветовой скоростью, а со скоростью обычного канала связи.

Сравнивая свои результаты измерений с результатами измерений отправителя, получатель может прочесть сообщение: если знаки проекций спинов для данного номера измерения (скажем, в десятом измерении) совпали, то это ноль, а если они противоположны то это единица.

И даже если сообщение по обычному каналу связи будет перехвачено, это не страшно.

Ведь у перехватившего разговор нет записей получателя.

Как видно из предшествующего раздела, для создания квантового канала связи достаточно источника ЭПР-пар частиц и двух измерительных проборов-приемников.

Но в этом случае человек, создающий запутанные пары, знает текст передаваемого сообщения, ведь он создает «нули» и «единицы» в соответствии с текстом послания. А можно ли использовать квантовый канал связи так, чтобы создатель ЭПР-пар частиц (назовем его С) был не в курсе передаваемого сообщения? Оказывается да.

Опишем идею такого процесса, предложенного в работе [9]. Пара, состоящая из двух ферми-частиц со спином, находится в состоянии, волновая функция которого может быть представлена, как суперпозиция следующих четырех состояний

$$\Phi^{\pm}_{1,2} = \left(\frac{1}{\sqrt{2}}\right)\left(\left|\uparrow_1\right\rangle\left|\uparrow_2\right\rangle \pm \left|\downarrow_1\right\rangle\left|\downarrow_2\right\rangle\right), \quad \Psi^{\pm}_{1,2} = \left(\frac{1}{\sqrt{2}}\right)\left(\left|\uparrow_1\right\rangle\left|\downarrow_2\right\rangle \pm \left|\downarrow_1\right\rangle\left|\uparrow_2\right\rangle\right)$$

Пусть С создает ЭПР-пары в состоянии .

Первая частица пары поступает к отправителю сообщения (обозначим его А) (рис. 3). Он добавляет к ней третью частицу, такую же, как и частицы пары, в состоянии

$$\psi_3 = \alpha\left|\uparrow_3\right\rangle + \beta\left|\downarrow_3\right\rangle, \quad |\alpha|^2 + |\beta|^2 = 1$$

.....

$$\begin{array}{l}\Psi_{1,2,3} = \frac{1}{2}\left\{\left(-\alpha\left|\uparrow_2\right\rangle - \beta\left|\downarrow_2\right\rangle\right)\Psi^{-}_{3,1} + \left(-\alpha\left|\uparrow_2\right\rangle + \beta\left|\downarrow_2\right\rangle\right)\Psi^{+}_{3,1}\right. \\ \left. + \left(\beta\left|\uparrow_2\right\rangle + \alpha\left|\downarrow_2\right\rangle\right)\Phi^{-}_{3,1} + \left(-\beta\left|\uparrow_2\right\rangle + \alpha\left|\downarrow_2\right\rangle\right)\Phi^{+}_{3,1}\right\}\end{array}$$

производит над прилетевшей частицей соответствующее преобразование (оно зависит от номера, но не зависит от и) и получает клон третьей частицы.

В случае фотона это достигается набором полуволновых пластин.

В случае электрона можно использовать импульс магнитного поля.

При этом С не имеет представления о полученной В информации. Явление возникновения в результате ЭПР-процесса клона частицы отправителя получило название «квантовая телепортация».

В этом процессе отсутствует телепортация материи, передается только информация. Вернемся теперь к квантовому каналу связи.

Можно выбрать третью частицу в состоянии с для передачи нуля, а в состоянии - для передачи единицы.

Измеряя проекцию спина полученного клона на выделенную ось, B получает бит информации. Экспериментально процесс квантовой телепортации осуществлялся неоднократно различными группами ученых.

В 2012 г. китайскими учеными была осуществлена телепортация фотонов в атмосфере на расстояние около 100 км [10]

Теория квантовой телепортации

(потом посмотрю, мб расширю раздел этот)
просто знаю, что начинать нужно с википедии
и тут много таких прямо интересных глав.

27.6 Quantum Theories that are Considered to be Bad or False

(когда буду на самом деле пользоваться записей, полезный очень будет раздел, пока - на всякий случай просто создан.)

27.6.1 Introduction to Matrix Mechanics

(нужно будет, тут поизучаю)

27.6.2 Other Theories

(всё остальное тупо сюда собираю и всё)

Квантовая механика в многомерных пространствах

(потом подумаю мб про это, пока что не до этого)

Реляционная квантовая механика

хз зачем, но такое есть

альтернативные квантовые теории

разумно и достаточно строго обсудим их.

Теория Гирарди — Римини — Вебера

(Пока из Википедии и не нужно было ни разу)

обзор

как типа неработающая теория, но такая есть, так что и я немного скажу про нее

Теория Гирарди — Римини — Вебера или теория ГРВ (англ. Ghirardi — Rimini — Weber theory, GRW) — одна из теорий объективного коллапса волновой функции в квантовой механике. Теория пытается решить проблему измерения и восполнить пробел в копенгагенской интерпретации, ответив на вопрос, как происходит коллапс волновой функции.

Теория ГРВ отличается от других теорий объективного коллапса тем, что коллапс волновой функции происходит спонтанно, без вмешательства внешнего измерения. Такой подход даёт возможность решить проблему измерения, в частности ответить на вопрос, где и когда квантовая система, находившаяся изначально в состоянии

суперпозиции, переходит к однозначным результатам, наблюдаемым на макроскопическом уровне с помощью измерительного прибора.

Теория ГРВ была предложена в 1985 году итальянскими физиками Джанкарло Гирарди, Альберто Римини и Туллио Вебером[1][2].

формулировка

пока не актуально, но потом мб займусь.

мелкие странные интерпретации

у МГ иванова спишу их.
потом.

Новые теории мироздания

(потом подумаю мб про это, пока что не до этого)

Сознание человека с точки зрения квантовой механики

(мб когда-то почитаю про это, но это скорее всего бесполезное занятие)

27.6.3 Erroneous Understandings of Quantum Mechanics

(тут то, как не нужно учить квантмеху!!! соберу, почему это так, укажу, как нужно. а то много путаниц тут тоже! со временем.)

27.6.4 On Quantum Cosmology (??)

(?? нужно писать вообще её сюда или нет?)

27.6.5 On Multiverses

27.6.6 On Hidden Variables Theory

(???)

Проверка неравенств Белла

Part VIII
Appendix

A Introduction and Overview of Quantum Mechanics

A.1 More Motivation for Quantum Mechanics

A.1.1 Other General Motivation

Квантовая механика - один из фундаментальных разделов физики

Квантовая физика - важнейший предмет физики, потому что почти каждый раздел в нее упирается, использует ее.

Формирование картины мира

Квантовая механика как прекрасно формирует картину мира, так и прекрасно разрушает различные заблуждения о том, что есть квантовый мир.

Такое видение в долгосроке может очень сильно повлиять на различные действия.

Можно строить квантовые компьютеры

это востребовано в мире

Это крутая вещь.

только этим отдельно нужно заняться, если отдельно не засиживаться в этом направлении, то толку от таких возможностей нет.

но у меня есть глава про них, ибо она очень и нужна.

(укажу, как начать в них разбираться и как выйти на исследования. ссылки на статьи или организации, которые этим занимаются)

Можно заняться квантовой оптикой

это востребовано в мире

(укажу, как начать в них разбираться и как выйти на исследования. ссылки на статьи или организации, которые этим занимаются)

Можно понять, как на самом деле атом устроен

(разве что полно принципиальных сложностей, но по идее в это тоже можно пойти)

Можно попробовать исследовать наше сознание

потому что где-то в мозгу если душа и есть, то она точно будет находиться в месте, описываемом квантовой механикой.

(пока не до этого)

Удивительные факты квантовой механики

(тут многие есть опыты, которые я почти готов описать, но о них сперва в самой записи напишу)

Удивительные совпадения

The most exact value for the ratio of proton to electron mass is $1836.12 \approx 0.05$. It may be of interest to note that this number coincides with $6\pi^5 \approx 1836.12$.

(энергия связи электрона и время жизни вселенной (??? напишу потом))

Квантовая механика контринтуитивна (????)

(раскрою тут эту мысль, почему так. пока не могу, потому что не засиживался в научпоп, потом когда-то подумаю про это)

Результаты квантовой механики

(самые принципиально необъяснимые и важные тут напишу, всякие второстепенные эффекты не буду указывать тут.)

Объяснены спектры атомов

(тут формула, почему они на самом деле есть)

Польза для развития

Обсудим пользу для общего саморазвития и для развития как физика.

(выделю потом главное, пока я хз, про что стоит писать, а про что нет. что там с мировоззренческим развитием??? его что-то мало кто получает.)

Квантовая механика может хорошо тренировать прикладную и фундаментальную математику

Это тоже очень важно, потому что часто очень нужны некоторые математические функции, методы комплексного анализа и дифференциальных уравнений, так что потренироваться в них и объединить в одну теорию очень круто с помощью квантовой механике.

Потом смотришь - в самых разных разделах и используются эти методы, что тоже круто.

Прикладная:
- методы точных решений диффуров
- методы приближенных решений диффуров
- численные методы

фундаментальная:
- Можно собрать функан параллельно, если заниматься строгой квантовой механикой

О том, как меняются взгляды на мир, когда занимаешься квантовой механикой

(укажу их, акцентируя мотивацию к квантмеху)

A.1.2 Motivation for Sections of Quantum Mechanics

Польза квантовой механики для общества

(тут подумать нужно, но такой вопрос тоже часто может возникнуть у тех, кто не в науке)

Изучив квантовую механику, будет что ответить эзотерикам

Потому что полно людей, которые верят в мистику и магию, при этом иногда приплетают физику, причем чаще всего квантовую.

Мотивация к феноменологической квантовой физике

основы квантовой механики принципиально объясняют суть природы и физики

связь с классической механикой, наблюдения...

Можно четко понимать, почему иные описания неверные

Если свой способ описания есть, то другим теориям уже верить не будешь. Что сути прочищает разум. Наверное..

Мотивация к типичным частям квантовой механики (?)

мотивация изучать модели рассеяния

вроде много где они нужны, но это не точно.

Мотивация к строгой квантовой механике

Возможность понять что-то хотя бы в какой-то степени нормально

Полностью квантовую механику мало кто может понять, разве что, возможно, специалисты. Тем же, кто решил за 3 месяца понять ее, занимаясь только этим вопросом и оставив занятия по изучению ее методов и приложений, тому только и остается, что открыть книгу с математической стороной. Темы с физической стороной и следствиями сути квантовой механики не научат. Конечно, математическая книга тоже может мало помочь понять, но точно - это то, с чего следует начинать, чтобы заложить хороший фундамент.

Исчезновение путаницы в общей картине квантовой физике

Если делать нестрого - то непонятно вообще, что и почему там есть. Строгий подход поможет всё собрать в связанную картину.
(так говорят, вроде такое может и быть.)

Развитие способности четко определять понятия, с которыми мы работаем

без строгого подхода тут не уехать.

Может быть, какие-то задачи можно решить, которые с нестрогим подходом не будут решаться (??)

(пока с этим хз)

Мотивация к квантовой теории информации

Наиболее известно приложение квантовой механики - это квантовые компьютеры. Обсудим, зачем этим заниматься, потому что скорее всего занятие квантовыми компьютерами будет самое полезное и дающее больше всего результатов.

Квантовые компьютеры востребованы в мире

то се, все говорят про это.

Изучая квантовую теорию информации, можно некоторые важные темы понять очень строго

То есть по сути нормально разобраться в предмете, что очень сложно сделать, без строгого подхода.

(конечно, речь о том, что преподаватель тоже хороший. но это большая мотивация потратить пару недель на это направление)

Многие лучшие ученые мира занимались квантовыми компьютерами

Фон Нейман, Фейнман, Тьюринг, т.п.
Так что тоже хочется этот путь пройти.

Мотивация к другим разделам квантовой механики

мотивация изучать ядерную физику

???? вроде это и круто, вот только мы простейшие модели будем понимать, а то, что в реальности происходит - другой вопрос.

так что толку от простейших моделей?

плюс они кстати сложные и требуют отдельного времения.

Глубокое понимание, что такое ядро и что внутри

и так можно лучше понимать природу. Только вот займет это уж очень много времени.

Можно понимать как работают ядерные реакторы

Разве что все равно пользы не много от этого будет, потому что к реакторам не допустят, если ты не специализируешься на ядерной физике.

A.2 How Professionals in Quantum Mechanics Think?

Обсудим подробно мышление профессионалов в квантовой механике.

A.2.1 Useless and Useful Parts of Quantum Mechanics

(discuss, which are which)

A.2.2 Approaches for Description of Quantum Phenomena

Отношение к квантовой механике

Квантовая механика как в первую очередь пара уравнений и их решений, во вторую уже - понятия и построения ее

(именно этот подход для теормина оказывается самый годный. мб он вообще почти всегда годный. потом подумаю про это. стоит ли вообще думать про нюансы ее построения и определений, если это вообще не нужно? пока думаю, что просто нужно заботать модели, потом уже задаваться идейными вопросами.)

квантовая механика как аппарат, который можно применять к другим разделам физики

То есть квантовая механика именно способ, причем совершенный.
(интересный взгляд, созрею - обсужу, насколько он верен. Слепо верить, что это так не считаю нужным.)

доказательство совершенности квантовой механики в двух словах

часто так говорят, Вайнберг доказал, я мб тоже это когда-то посмотрю.
пока так, чисто заготовка.

О том, что в квантовой механике нет ничего контринтуитивного

(часто говорят, что есть, тут обосную, почему это не так.)

Квантовая механика как загадки и разгадки

именно так к этому и нужно относиться.
а то можно утонуть в формализме.

Are big books of QM meaningful?

(currently, I think that often - no. discussion of models and methods is made just to avoid attention from the fact that we don't know how nature works. i am not sure. I'll write later, is a big discussion of methods and models are worth at all our attention? maybe yes, for applications...)

Как понимать классическую механику, чтобы догадаться до квантовой механики? (!?!??!??)

(очень важный вопрос для профессионализма, продумаю потом!!)

What is finally going on with the idea "I want to understand life around me better, so I'll start with fundamental microscopic quantum mechanics"?

Same idea is "to speak better with people, I'll learn quantum communication and will be the top world speaker".

So, currently, I think that this is just a dead end. One would not understand anything in the world better.

The moral of the story that 21st century physics still have no answers about the real life, only about some specific setups (however, there are a lot of them and it is still a big progress of humanity).

(???? or there is something, which QM really teaches us??? I'll think later)

Типичные неверные понимания квантовой механики

представление, что соотношение неопределенностей имеет отношение к происхождению волновой функции

Вспомним вывод волновой функции....

Некоторые утверждают, что мы не можем точно измерять параметры частицы, поэтому возникают волновые функции.

К сожалению, такие взгляды обречены на неудачу, в самом деле

...

Поэтому

"частица и волна одновременно"

ух, типичное дело.

"волна материи"

соотношение де бройля такое не простое, что его можно по-разному трактовать.

Думать, что каноническое квантование и вторичное это разное

(Вообще не актуально, но Володя говорил, в П Ш написано, мб посмотрю.)

О строгой квантовой механике

О необходимости математической подготовки по многим фронтам

без нее нормально не поймешь.

но стоит ли она того? пока думаю, что нет, ибо заморочек много, а обойтись без нее тоже вроде еще как можно.

Но это большая проблема, потому что нормальная подготовка к строгой квантовой механике - отдельное занятие на месяц как минимум.

(мб когда-то займусь этим, вряд ли скоро)

О том, что в ней нет физики

Пока в точности так и думаю. а где она там? какие-то свойства операторов.

Может, стану лучше разбираться - что-нибудь скажу про это другое.

Так всё-таки, можно ли понять квантмех? (???????)

Распишу ответ про это. Все это упирается в разделы что такое волновая функция или что такое матрица плотности? . Один из первых пар в мышлении профи.

Чтобы выучить квантовую механику нужно мыслить по-квантовому. Что это значит?

(конечно, это больше шутка, но в качестве шутки тоже можно придумать интересные соображения. подумаю потом когда-то.)

О строгом математическом подходе

О том, когда он нужен, а когда нет

(тут порассуждаю об этом, большой вопрос.)

О том, почему в жизни никто строгим подходом не пользуется

Нпр психология, размышления о жизни - у людей нестрогий подход и они даже не думают как-то его делать более строгим. Порассуждаю, почему в квантовой физике мы внезапно так меняем подход.

О важности математики для квантовой механики

(тут рассуждения про то, насколько вообще её нужно знать? и что нужно из неё знать. тоже много порассуждать можно. Думаю, малого раздела должно хватить, если не хватит - расширю!)

О применениях квантовой механики (??)

Укажем, какие самые полезные темы в квантовой механике, как они приеменяются в других разделах физики и других науках.
(пока фоном ищу ответы. потом очень четко укажу все применениях, которые знаю!!)

обзор того, что квантовая механика дает теории электричества

где она там нужна?
что с ней делать можем новое?

квантовая механика в космологии

мб как раз про связь с линзированием и напишу тут?

Обзор применения в финансах

хз, там континуальный интеграл используется.

обзор применений интеграла по траекториям

О важности раздела про матрицу плотности и открыте системы

(мб это и очень важный раздел, но порассуждать про это нужно.)

обзор применений квантовой физики в астрономии

Что есть знать квантовую механику? (?)

(напишу потом ответ на этот вопрос, пока не уверен. думаю, обычные 2 семестра квантмеха + 1 семестр общефиза. Если пройти без скатывания, то этого и можно считать, что основы изучены. Если катка была, то не нужно переделывать.)

О выборе тем в квантовой механике

(сперва выбрать нужно, на чем сосредоточимся?)

О важности изучения задач рассеяния

(ну окей, вот ямы, так рассеивается, зачем вообще на это тратить время? тут ответ, пока занимаюсь этим, ибо тренировка хорошая)

Необходимые предметы для квантовой механики

Хорошие основы классической механики

Она очень важна.
(потом раскрою)

Хорошие минимальные основы математики

(потом раскрою, что общие основы тут используются, а также потом в строгий квантмех переход может быть, если они будут нормальными.)

Дополнительные предметы для квантовой механики

Функциональный анализ

ибо там большая тусовка, которая на этом языке всё и описывает.

Wolfram/ Другой язык программирования

Потому что многое хочется вычислять и моделировать, так что очень уж он будет кстати.

Типичные заблуждения про изучение квантовой механики

Обсудим то, что не следует делать при изучении квантовой механики, ведь иначе можно уйти в тупик, из которого выход будет месяцами длиться.

(самую суть именно про квантмех укажу. с опытом очень важных выводов будет много, пока особо исследованиями не занимался.)

Не следует во время изучения квантовой механики общаться с мало знающими в ней о ней

Если общаться о ней с теми, кто не владеет ей без сформированной своей картины происходящего, то очень легко подцепить тупиковое мышление, с которым изучение и закончится. Поэтому если человек не признанный авторитет в квантовой механике, то

не следует свободное время с ним проводить за общением о ней. Только после сформированной своей картины мира такое общение не будет вредить.

А именно, не следует общаться со студентами, с прочитавшими популярные книги, а особенно - с уверенными в эзотерических концепциях. Особенно не следует общаться с теми, кто понял пару конструкций квантовой механики, научился их рассказывать, при этом отрицает многое также присутствующее в этом предмете. Такие могут на месяцы увести развитие не в ту сторону, так что их очень важно стороной обойти.

(в пример Володю приведу мб чтобы четко указать, что общение с ним замедлит развитие на пару месяцев на пустом месте, и хотя что-то и даст, это будет совсем не то, что на самом деле нужно. пока плохо раскрыл, почему так не следует делать.)

Не следует общаться с экспериментаторами, не овладев теоретической базой

Так следует делать тому, кто хочет стать мастером в квантовой механике. Предмет слишком большой, чтобы одновременно и теоретическую и экспериментальную части изучать. Сперва пройти минимальную теоретическую нужно, потом уже эксперименты изучать.

(проверю с опытом такую точку зрения.)

Не следует начинать математический подход изучать без теоретической и экспериментальной базы

Потому что зависнешь в математике раньше времени. Физику куда проще изучить, чем пройти все математические концепции. Да и потребность в них возникает только тогда, когда сам по себе предмет изучен и есть навыки хотя бы простейшие эксперименты описывать.

Многие считают иначе, моё мнение по поводу них: они лгут.

A.2.3 On Studying Quantum Mechanics

Об общефизическом подходе к изучению квантовой механики

Про него многие говорят, причем в негативном ключе, поэтому приведем свои небольшие соображения.

Общефизический подход хорош для кругозора

Это только про него думаю.
с опытом уточню.

Общефизическая квантовая физика имеет особенности, но берется обычным образом

общая квантовая физика большая, много деталей имеет и пока не будет четкой теории квантовой механики, будет казаться, что мало связок в них, тем не менее, работаем как обычно.

Всё по тем же давно понятным методам, спокойно всё изучается. Кто не может - тот просто не умеет учиться, ну или обстоятельства появились, что редко бывает.

Сложностей с ним нет, однако есть многие другие вопросы.

О проблеме общефизического подхода в преподавании

Просто Овчинкин, как и многие другие, объясняет супер кончено и так, что проще самому решить. Вот и очень большой фактор, почему общефизом мало кто занимается, потому что подача просто конченная, это очень раздражает. Не следует забывать этот фактор, он среди решающих.

Насколько те или иные темы важно изучать?

(порассуждаю, насколько нужно вообще мастерить 1Д рассеяние через точнорешаемые потенциалы и все такое. ПТФ вставляет в курс свой, но это очень спорно. Потом подумаю, пропишу, стоит ли это того? Думаю, что точно тому, кто не владеет общими соображениями про основы, а также не имеет отлично выученный какой-то сложный предмет, чтобы в принципе уверенным быть в своих силах изучать большие темы - нет, не стоит того фокусироваться на эти темы.)

A.2.4 Ways to Earn Money by Knowing Quantum Mechanics (!!)

(!! накидаю вскоре!)

Устроиться в компанию, занимающейся квантовыми вычислениями

(и в этом случае открывается просто новая большая сфера квантовой информатики, так что нужно быть готовым а неё погружаться. Для меня это такой себе вариант, потому что это не самый приятный раздел квантовой механики, скорее задротский и математический)

Плюсы:

Минусы:

- это вмеру скучно. Есть разделы интереснее

Делать популярные видео о квантовых явлениях

A.2.5 People, Who Are Engaged in Quantum Mechanics

(write who are they, what are known about them? not all people are doing QM and are capable for it. psychological features)

Вопросы на проверку тем, кто говорит, что знает квантовую механику (?!)

(потом соберу интересные, пока не очень понимаю их.)

Расскажите о теореме Вигнера-Эккарта

(пока прикол в том, что там все супер детальное, так что очень многое видно, если человек про нее будет рассказывать.)

A.2.6 Use of Quantum Mechanics in Everyday Life

Укажем, как квантовая механика используется в обычной жизни

A.2.7 Ways to Guess the Main Ideas of Quantum Mechanics

незаменимая часть нормального понимания предмета.

В чем были основные ошибки и непонимания ученых в прошлом, когда не было КТП и до этих методов не могли догадаться? (!?!??!??!?)

(для профессионального уровня очень важно ответить на этот вопрос подробно!!)

Способы догадаться до основных концепций и идей квантовой механики (???)

(для профессионального уровня очень важно ответить на этот вопрос подробно!!)

Способы догадаться до основных уравнений (???)

хз

способы догадаться до экспериментальных методов проверки квантовой механики

я хз и как проверять и как догадываться до нее.

A.2.8 Influence of Quantum Mechanics on Worldview

(пока я слишком плохо её понимаю, чтобы говорить об этом, потом подумаю. Много про это также написано, в том числе в научпопе.)

Обсудим вкратце, что говорит нам квантовая механика про то, из чего состоит мир.

Подробнее это описано в разделе про философию в конце записи, а еще более подробно - в отдельной записи про философию.

A.2.9 Overview of Special Applications of Quantum Mechanics (???)

(just general overview what to do and why?)

Квантовая механика для промышленности

(укажу, где она нужна, что с ней можно сделать? пока не знаю, и это проблемка)

A.2.10 On Dead Ends in the Creation and Understanding of Quantum

Квантовая механика интересна тем, что многие, кто ее изучают, могут нести лютый бред в плане различных интерпретаций. Еще больший бред можно услышать от тех, кто о ней что-то слышал. Соберем разные такие утверждения не чтобы поржать, а чтобы лучше понимать, какова на самом деле суть квантовой механики.

A.3 Acknowledgements

Currently, no one except me has worked on the sections of this note (with the exception of sections taken from books).

A.4 Literature

Обсудим литературу по квантовой механике, из которой создана эта запись.

(потом структуру улучшу, пока почти рандомно все книги записаны после самых основных)

A.4.1 Main Literature

Basic educational literature

David Tong: Lectures on Topics in Quantum Mechanics

Лекции, в которых много основ изложены, отлично для начала. Кстати, кто совсем не знает квантовую механику, может начать с "первой части" курса Tong-a "Lectures on Quantum Mechanics", просто спустя время эта запись кажется очень известной и поврехностной. А вот лекции по отдельным темам - там есть, что почитать, о чем подумать, и к чему вернуться чуть что.

Masatsugu Sei Suzuki Lecture Notes on Quantum Mechanics II https://bingweb.binghamton.edu/~suzuki/QuantumMechanics2.html

Набор очень хороших и подробных лекций про разные модели. Много тем разобрано, написаны без желания сэкономить место. Очень приятно читать и очень много полезной информации.

[1] Побойко И., Антоненко Д., Степанов Н. Семинары по квантовой механике в институте Ландау

Короткий конспект пары хороших методов, про которые очень много времени ушло бы самому вычитывать в книгах. Однако, некоторые разделы написаны абсолютно нечитаемо, видимо, один из авторов абсолютно не умел писать своё понимание темы.

Мигдал Крайнов Качественные методы в квантовой теории

Очень крутая книга на 150 страниц, которая очень многому учит, так что обязательная для понимания происходящего.

[2] Griffiths, D. J., Schroeter, D. F. Introduction to Quantum Mechanics

Wonderful and famous book that covers all basic topics. Also, see solutions to it https://stemjock.com/griffithsqm3e.htm TODO: add very good problems from it (after I finish doing problems which I already started).

[2] Griffiths, D. J. Solutions to Introduction to Quantum Mechanics 3e https://stemjock.com/griffithsqm3e.htm

Wonderful solutions, they will help a lot in understanding. Unfortunately, not all solutions are given in 2024.

[3] Киселев Квантовая механика часть 1

Книга, по которой я учился. Очень много хороших тем, однако не везде изложение понятное и не все темы в ней важные для понимания.

[4] Киселев квантовая механика часть 2

Книга, по которой я учился. Очень много хороших тем, однако не везде изложение понятное и не все темы в ней важные для понимания. Некоторые темы вообще такие, про которые лучше не думать, потому что время впустую потратите.

[5] K. Zhou Lecture Notes on Undergraduate Physics

Great short notes about some parts of physics and with many sections about quantum mechanics.

[6] Кингсеп, А.С и др. Общая физика: квантовая физика и термодинамика

Обсуждается много вводных и простых тем в квантовой механике, можно во многом разобраться и почитать в меру подробные описания. Типичный вузовский российский учебник.

Карлов Н. В., Кириченко Н. А. Начальные главы квантовой механики. - М.: ФИЗМАТЛИТ, 2004. - 360 с. - ISBN 5-9221-0538-8.

Многие темы просто объяснены, типичная книга по общей физике, можно многому научиться.

Основные задачники

[7] (GKKG) Galitski, V.M. and Karnakov, B. and Galitski, V. and Kogan, V.I. Exploring Quantum Mechanics: A Collection of 700+ Solved Problems for Students, Lecturers, and Researchers

Основной задачник. Изучать из него задачи его следует 2/3 всего времени в первом цикле изучения квантовой механики. Конечно, она слишком большая, чтобы ставить целью изучить полностью, но многие задчи разобрать - крайне полезно и в других местах вообще не написаны они.

(ГК) Гольдман Кривченков Сборник задач по квантовой механике

Очень крутые задачи, решение многих приведено, книга номер 1 по изучению квантмеха. Однако некоторые задачи очень непонятны, так что иногда хочется просто открыть другую книгу.

[8] (Б) Белоусов задачник по теоретической физике

Неплохие элементарные задачи, но их очень мало.

Основная профессиональная литература

[9] Тахтаджян Л. А. Квантовая механика для математиков

Прекрасная книга для понимания математической квантовой механики. Хотелось бы разве что больше примеров и больше связей с не математической квантовой механикой, но уже с ней очень многое можно понять.

[10] Зинн-Жюстен, Жан Континуальный интеграл в квантовой механике

самая прекрасная книга, по которой и буду создавать изначально запись. книга настолько прекрасна, что ничего другого перед ней читать не хочу! и уже многее выгрузки по ней сделаны!

[11] Michael A. Nielsen, Isaac L. Chang Quantum Computation and Quantum Information

Большая, очень известная книга про квантовую теорию информации.

[12] А. И. Базь, Я. Б. Зельдович, А. М. Переломов Рассеяние, реакции и распады в нерелятивистской квантовой механике

Хорошая полезная книга, 500 страниц только теория рассеяния, нужно будет - скорее всего основной книгой и будет.

A.4.2 Additional Literature on Basic Topics

Literature with detailed explanations

Wheeler's notes https://www.reed.edu/physics/faculty/wheeler/documents/
Notes by a pure genius, well-written and very informative. I would even pay 200 euros to have them, but I am not sure that they are really used for the research, just for general education. Later, I'll add all of this to my notes.

Suzuki's notes https://bingweb.binghamton.edu/~suzuki/index.html
Also, a lot of notes by a pure genius, well-written and very informative. I would also even pay 200 euros to have them, but I am not sure that they are really used for the research, just for general education. Later, I'll add all of this to my notes.

Литература о профессиональных методах

Зайцев Р.О., Михайлова Ю.В. Метод вторичного квантования для систем многих частиц
Подробная методичка про вторичное квантование, давно в планах продумать её.

[13] Ландау Квантовая механика
Хорошая книга, много полезного, но гораздо легче утонуть в объеме, чем получить пользу, так что ее читать лучше только после основных. В целом, ничего супер важного там нет, чего в других не рассказано, тем не менее, раз в своей жизни неделю глубоко думать о ней, будучи готовым к ней, очень полезно.

По математике и начальной физике в помощь

Нейман Математические основы квантовой механики [1964]
Хз.
Вейль
вроде вымерло, но тоже интересно почитать, теорию групп прокачать бы сперва!

Статьи, раскрывающие углубленный подход к квантовой механике

[14] Alireza Behtash, Gerald V. Dunne, Thomas Schafer, Tin Sulejmanpasic, Mithat Unsala, Toward Picard-Lefschetz Theory of Path Integrals, Complex Saddles and Resurgence
Крутая статья на 100 страниц со многими деталями. как теоретический подход профессиональный дается, так и много иллюстраций. Так что основы квантовой механики будут созданы со многими из нее идеями, по сути это известные идеи, подача просто мне нравится. вроде должно получиться.

[15] Kleinert, Hagen Path integrals in quantum mechanics, statistics, polymer physics, and financial markets
1600 страниц наверное шикарного текста, который наверное возьму в основу этой записи.

[16] Дирак П. Лекции по квантовой механике
искривленные пространства там тоже есть, так что интересная книга. 100 страниц - круто, почитаю потом.

[17] Tomonaga, S., The Story of Spin

Очень много есть информации про спины, про их открытия, про историю. Если очень интересует этот вопрос, то, возможно, одна из лучших книг для ответа на него. Узнал о ней из лекций L. Paolasini по магнетизму.

Профессиональная литература по атомной и ядерной физике

[18] Соловьев В. Г. Теория ядра. Модели ядер

говорят, крутейшая книга по ядерке. после общефиза могу попробовать, пока что скорее всего не скоро дойду до этого, ибо не актуально.

[19] Бор О., Моттельсон Б. Структура атомного ядра т. 1

Говорят, крутая очень книга по ядерке, пока что не до нее, но, возможно, очень много буду ее смотреть, потому что интересно.

[19] Бор О., Моттельсон Б. Структура атомного ядра т. 2

тут, наверное, жесткая ядерка, мне даже представить сложно, что там. по сравнению с этой книгой, такое чувство, что я знаю ядерку на нуле.

Бете Г. Элементарная теория атомного ядра

Может, потом почитаю, похоже на заморочку на минимум в пару недель, пока нет в этом потребности.

Мигдал А. Б. Теория конечных ферми-систем и свойства атомных ядер. - 2-е. изд.

мб добавлю

Ситенко А. Г. Теория ядерных реакций.

говорят, жесткая книга. так или иначе, не до нее.

Notes and references about classical mechanics by Takhtajayan

Classical references are the textbooks [Arn89] and [LL76], which are written, respectively, from mathematics and physics perspectives. The elegance of [LL76] is supplemented by the attention to detail in [Gol80], another physics classic. A brief overview of Hamiltonian formalism necessary for quantum mechanics can be found in [FY80]. The treatise [AM78] and the encyclopaedia surveys [AG90], [AKN97] provide a comprehensive exposition of classical mechanics, including the history of the subject, and the references to classical works and recent contributions. The textbook [Ste83], monographs [DFN84], [DFN85], and lecture notes [Bry95] contain all the necessary material from differential geometry and the theory of Lie groups, as well as references to other sources. In addition, the lectures [God69] also provide an introduction to differential geometry and classical mechanics. In particular, [God69] and [Bry95] discuss the role the second tangent bundle plays in Lagrangian mechanics (see also the monograph [YI73] and [Cra83]). For a brief review of integration theory, including the Riesz-Markov theorem, see [RS80]; for the proof of the Gelfand-Naimark theorem and more details on $\mathbb{C}^*$-algebras, see [Str05] and references therein.

Our exposition follows the traditional outline in [LL76] and [Arn89], which starts with the Lagrangian formalism and introduces Hamiltonian formalism through
the Legendre transform. As in [Arn89], we made special emphasis on precise mathematical formulations. Having graduate students and research mathematicians as a main audience, we have the advantage to use freely the calculus of differential forms and vector fields on smooth manifolds. This differs from the presentation in [Arn89], which is oriented at undergraduate students and needs to introduce this material in the main text. Since the goal of this chapter was to present only those basics of classical mechanics which are fundamental for the formulation

of quantum mechanics, we have omitted many important topics, including mechanicalgeometrical optics analogy, theory of oscillations, rotation of a rigid body, perturbation theory, etc. The interested reader can find this material in [LL76] and [Arn89] and in the above-mentioned monographs. Completely integrable Hamiltonian systems were also only briefly mentioned at the end of Section 2.6. We refer the reader to [AKN97] and references therein for a comprehensive exposition, and to the monograph [FT07] for the so-called Lax pair method in the theory of integrable systems, especially for the case of infinitely many degrees of freedom.

In Section 2.7, following [FY80], [DFN84], [DFN85], we discussed Poisson manifolds and Poisson algebras. These notions, usually not emphasized in standard exposition of classical mechanics, are fundamental for understanding the meaning of quantization - a passage from classical mechanics to quantum mechanics. We also have included in Sections 1.6 and 2.7 the treatment of the Laplace-Runge-Lenz vector, whose components are extra integrals of motions for the Kepler problem [24]. Though briefly mentioned in [LL76], the Laplace-Runge-Lenz vector does not actually appear in many textbooks, with the exception of [Gol80] and [DFN84]. In Section 2.7, following [FY80], we also included Theorem 2.19, which clarifies the meaning of the Jacobi identity, and presented Hamilton's and Liouville's descriptions of the dynamics.

Most of the problems in this chapter are fairly standard and are taken from various sources, mainly from [Arn89], [LL76], [Bry95], [DFN84], and [DFN85]. Other problems indicate interesting relations with representation theory and symplectic geometry. Thus Problems 2.12 and 2.20 introduce the reader to the orbit method [Kir04], and Problem 2.18 - to the method of symplectic reduction (see [Arn89], [Bry95] and references therein). Problems 2.21-2.23 introduce the reader to the theory of Lie-Poisson groups (see [Dri86], [Dri87], [STS85], and [Tak90] for an elementary exposition).

Notes and references from Takhtajayan's section about basics of quantum mechanics

Dirac's classical monograph [Dir47] is the fundamental text. Other classical references are physics textbooks [Foc78] and [LL58]. The monograph [Sak94] is a popular text for graduate courses in physics departments. Another useful physics reference is the encyclopedic treatise [Mes99], which discusses at length the origin of quantum theory and the development of its mathematical formalism. An elementary textbook [PW35] provides an introduction to the old quantum theory, including Bohr-Wilson-Sommerfeld quantization rules, and applications of quantum mechanics to chemistry. We refer the interested reader to these sources for physical formulation and the origin of quantum mechanics, including a discussion of basic experimental facts: the double-slit experiment and particle-wave duality. Quantum mechanics does not account for single measurement outcomes in a deterministic way, and the quantum process of measurement admits different interpretations. The accepted one is the so-called Copenhagen interpretation, in which a measurement causes an instantaneous "collapse" of the wave function describing the quantum system.

Monographs [Rud87, BS87, AG93], as well as [RS80, RS75], contain all the necessary material from the theory of operators in Hilbert spaces; the latter treatise also covers the theory of distributions, Fourier transform, and self-adjointness. The book [Kir76] introduces the reader to various methods in the representation theory, and the monograph [BR86], written for theoretical physicists, contains all the necessary information on the representation theory of Lie groups and Lie algebras. A succinct introduction to the method of stationary phase and other asymptotic methods is given in the classical text [Erd56] and in [Olv97]; see also Appendix B in [BW97]. Properties of Hermite-Tchebyscheff polynomials [29] can be found in the classical mono-

[024] We will see in Chapter 3 that these extra integrals are responsible for the hidden SO(4) symmetry of the hydrogen atom.

graph [**Sze75**], as well as in many other reference books on special functions and orthogonal polynomials.

Our exposition in Section 1.1 follows a traditional approach to the mathematical foundation of quantum mechanics based on Dirac-von Neumann axioms. These axioms go back to von Neumann's classical monograph [vN96], with more detailed discussion in [Mac04]; see also [BS91], notes to Chapter VIII of [RS80], and references therein. Another mathematical description of quantum mechanics is based

on $\mathbb{C}^*$-algebras and the Gelfand-Naimark-Segal reconstruction theorem, and can be found in [**Str05**] and references therein.

Our exposition in Section 2 follows the outline in [FY80]; see [Ber74] for the general mathematical formulation of the quantization problem and the recent survey [AE05]. Having in mind a more advanced audience than for [FY80], in Sections 2.1 and 2.2 we included a complete mathematical treatment of Heisenberg commutation relations and coordinate and momentum representations. In Sections 2.2 and 2.3 we use the same normalization of the eigenfunctions of continuous spectrum as in [Foc78]; it corresponds to the orthogonality relation in Section 2.2 of Chapter 3. In our exposition in Section 2.6, which is otherwise standard, we include a proof of the completeness of the eigenfunctions $\psi_n(q)$, which is usually only mentioned in the physics textbooks. Holomorphic representation in quantum mechanics was introduced by V.A. Fock in 1932 [Foc32], where the scalar product in $\mathscr{D}_n$ was given in terms of the orthonormal basis of monomials $f_m(\boldsymbol{z})$. In terms of the integral (2.52) this scalar product was defined by V. Bargmann [Bar61]; holomorphic representation is also called Fock-Bargmann representation. Discussion of Wick symbols of operators in Section 2.7 essentially follows [BS91]; more details can be found in the original paper [Ber71b]. The method of geometric quantization is only briefly mentioned in remarks in Sections 2.2 and 2.7 ; the interested reader is referred to monographs [GS77, Woo92], lecture notes [SW76, BW97] and the survey [Kir90].

Our proof of the celebrated Stone-von Neumann theorem in Section 3.1 essentially follows the original paper of von Neumann [vN31]. The main instrument of the proof - the Weyl transform - was introduced by Weyl in the classical monograph [Wey50] (see [Ros04] for the history and generalizations of the Stonevon Neumann theorem). Invariant formulation of the Stone-von Neumann theorem, discussed in Section 3.2, as well as the relation with the triple Maslov index, methaplectic group, Shale-Weil representation, and applications to number theory, can be found in [LV80]. We refer to [BS91] for the extended discussion of $\boldsymbol{pq}$ and $q\boldsymbol{p}$-quantizations as their relations with the Weyl quantization, as well as for more details on the $\star$-product, introduced in Section 3.4. The beautiful formula (3.24) for the $\star$-product - composition of the Weyl symbols - belongs to Berezin [Ber71a].

The notion of the deformation quantization was introduced in [**BFF$^+$78a**, **BFF$^+$78b**], where the solution of Problem 3.12 can be found. The fundamental theorem that every Poisson manifold admits a deformation quantization was proved by Kontsevich in [Kon03]. More on Hochschild cohomology and the deformation theory of associative algebras can be found in the survey [Vor05] and references therein. The deformation theory point of view on the evolution of physical theories, like a passage from classical mechanics to quantum mechanics emphasized in Faddeev's lectures [FY80], can be found in [Fla82] and [Fad98].

Most of the problems in this chapter are rather standard and are mainly taken from the references [RS80, BS91]. Other require more sophistication and are aimed at introducing the reader to a new topic. Thus the asymptotic expansion in Problem 2.11, which can be found in monograph [Sze75], is an example of semi-classical asymptotics, and Problem 3.1, taken from [Nel59], gives a criterion when the irreducible unitary representation of the Heisenberg algebra is integrable. Problems 3.17-3.19 introduce the reader to the theory of quantum groups (see

[029] Following V.A. Fock [Foc78], in Section 2.6 we used the more appropriate name Hermite-Tchebyscheff polynomials instcad of the customary Hermite polynomials (see [Ger50] for the relevant historic arguments).

[Jim85, Dri86, Dri87, RTF89]) and are taken from [Dri83] (see also [Tak90]). The fundamental result that every Lie-Poisson group admits a deformation quantization described in Problem 3.18 has been proved in [EK96] (see also [Enr01]).

4. Notes and references about spin, spinors

The notion of electron spin is fundamental for the agreement of quantum mechanics with experiments. See [Mes99] for a thorough discussion of the principal evidence supporting the hypothesis of electron spin (Zeeman effect, Stern-Gerlach experiment). Classic texts [LL58, Foc78] also introduce the concept of spin from a physics perspective. Representation theory of the Lie group SU(2) - the simplest compact non-abelian Lie group - is discussed in detail in [Vil68]; for the description of all irreducible representations of U(n) see [FH91]. Our discussion of the Pauli Hamiltonian in Section 2.1 follows [Foc78]; the case of a particle in a uniform magnetic field in Section 2.2 was first considered by L.D. Landau in 1930 (see [LL58]). Problem 2.2 shows that in the presence of a magnetic field the operators
X_0 and Y_0, associated with coordinates of classical trajectories of a charged particle, do not commute and cannot be measured simultaneously.

The Pauli wave equation in Section 2.1 is non-relativistic, i.e., it does not take into account the postulates of special relativity. The correct quantum description of the electron in an external electromagnetic field was proposed by Dirac and is given by the Dirac equation; the Pauli wave equation is obtained as its non-relativistic limit [Foc78]. The Dirac equation is a single particle equation which describes an electron and a particle with charge - e - a positron. In order to describe quantum processes of creation and annihilation of particles, one needs to pass from quantum mechanics to quantum field theory, which deals with systems with infinitely many degrees of freedom, and we refer to [IZ80] for an introduction.

The symmetrization postulate, formulated in Section 3.1, is another fundamental principle of quantum mechanics, and we refer to [Mes99] for its physical motivation. The N-particle Schrdinger equation describes all the properties of atoms. However, it is almost impossible to solve this equation analytically (for the potentials in atomic physics), and even numerically when $N > 2$; the case of the helium atom ($N = 3$) illustrates the difficulties of the problem. For this purpose various approximate methods like the one-electron approximation, the Hartree-Fock method and its modifications, have been developed (see [LL58, Foc78] for the details and [FY80] for a clear introduction). A correct description of the properties of atoms and an explanation of D.I. Mendeleev's periodic table of elements, based on these methods, has been a major triumph of quantum mechanics. For a detailed account we refer the interested reader to [LL58, Foc78] and [FY80]. The N-particle Schrdinger equation, in principle, also describes [5] all properties of molecules studied in chemistry. However, this "reductionism" does not work due to the complexity of the quantum N-body problem, and approximate methods like Hartree-Fock approximation play a central role in quantum chemistry.

The vector space $\mathbb{C}^2 \otimes \mathbb{C}^2$ describes the spin degrees of freedom of two electrons, and the spin states which are not represented as a tensor product $u \otimes v$ are called entangled. Entangled states are used to describe the Einstein-PodolskiRozen paradox, a quantum experiment, which apparently violates the principle of locality (see its description in [Bel87, Sak94]). The fact that quantum mechanics is correct and allows for an accurate description of the microworld is beyond any doubt, and is confirmed by numerous physical experiments. The Einstein-Podolski-Rosen paradox is only a "paradox" because classical intuition does not always correspond to the physical reality. Moreover, it follows from the Bell inequalities [Bel87] that any attempt to turn quantum mechanics into a deterministic theory by introducing the so-called hidden variables is fallacious; we refer to the web site http://en.wikipedia.org/wiki/EPR_paradox for further references. The vector space $\mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2$, describing the spin degrees of freedom of

several

identical particles of spin $\frac{1}{2}$, also plays a fundamental role in quantum computation theory. This is a rapidly developing field, and we refer the interested reader to the monograph [KSV02] for the mathematical introduction, and to the web site http://en.wikipedia.org/wiki/Quantum_computer for updates on the specialized literature. Another rapidly developing and exciting new application of quantum mechanics is quantum cryptography, reviewed at http://en.wikipedia.org/wiki /Quantum_cryptography.

Section 3.2 is a crash course on the representation theory of the symmetric group Sym_N - a beautiful piece of classical mathematics which has many interesting applications in modern combinatorics and representation theory. Our goal here was to give a concise and clear presentation of the basic necessary facts, and we refer to the classic text [Wey50] and to [FH91] for detailed accounts of representation theory, and to [GW98] for the Schur-Weyl duality. In Section 3.3 we emphasize the role of Schur-Weyl duality in studying the symmetry properties of coordinate wave functions. Physics textbooks like [LL58], [Dav76] and [Sak94] carefully treat the basic examples, but are somewhat vague in describing the form of the total wave function of N particles. The monograph [Foc78] is very precise in this regard, but in his presentation V.A. Fock is trying to reduce the usage of group theory to a minimum. Our goal in Section 3.3 was to fill this gap and to give a clear description of the symmetry properties of coordinate and spin parts of the total wave function by using the language of representation theory. For the case of N particles of spin $\frac{1}{2}$ this problem was solved by V.A. Fock in 1940; see [Foc78], as well as in yet another classic [Wig59]. For more applications of group theory to quantum mechanics we refer to the latter text, and to [Wey50].

Notes and references about Fermionic systems by Takhtajayan

Canonical anticommutation relations, discussed in Section 1, were introduced by P. Jordan and E. Wigner in 1928 [JW28]. We refer the reader to F.A. Berezin's classical monograph [Ber66] for a comprehensive mathematical treatment of canonical commutation and anticommutation relations. Though [Ber66] is mainly devoted to quantum systems with infinitely many degrees of freedom, which are studied by quantum field theory, it also discusses the simpler case of finitely many degrees of freedom. A self-contained mathematical introduction to Clifford algebras, their representations, and other topics can be found in [Var04] and references therein. The fundamental idea that systems with Grassmann variables appear as a semi-classical limit of fermions was formulated by I.L. Martin in 1959 [Mar59b, Mar59a]. Independently, F.A. Berezin in [Ber61] introduced Grassmann variables for rigorous mathematical description of the second quantization for fermion systems by using generating functionals for vectors and operators. Material in Section 2 - differential and integral calculus on the Grassmann algebra - belongs to F.A. Berezin, and our exposition follows [Ber66] and [Ber87]. The superalgebra - graded linear algebra - which we very briefly describe in Section 3, was also discovered and developed by F.A. Berezin [Ber87]. The references [Man97], [Fre99], and [DM99] provide the reader with a more abstract mathematical treatment, while lecture notes [Var04] supplement the category theory approach of [DM99] with
motivation from physics. We refer to [Ber61, Ber66] for the general discussion of the path integral over Grassmann variables, and of the matrix and Wick symbols of operators in the fermion Hilbert space. In Section 4 we follow the elegant exposition in [FS91]; as in Section 2.4 of Chapter 5, we carefully treat boundary conditions for Grassmann path integrals for the Wick symbols (as opposed to the formulas [Ber71a]).

[05] In this sense, quantum mechanics is a "theory of everything" for chemistry.

Notes and references about Schrodinger equation from Takhtajayan

The classical text [LL58] is the source of many basic facts on the Schrodinger equation, written from the physics perspective. The textbook [Foc78], another classic, shows meticulous attention to detail. There are numerous mathematics papers and monographs devoted to the different aspects of the Schrodinger equation, and here we mention only the sources being used. For the self-adjointness criteria in Section 1.1 we refer the reader to the encyclopaedia survey [RSS94] and to the treatise
[RS75], and references therein; in particular, in [RS75] one can find the proof that the Schrodinger operator for a complex atom is essentially self-adjoint. For the proof of Sears theorem, see [BS91]. Theorems 1.6 and 1.7 (the latter in the special case $V_1 = 0$) in Section 1.2 are proved in [BS91] and [RSS94]; see [RS78] for the proof of Theorem 1.7 in the general case, and for other generalizations. The proof of the Kato theorem can be found in [RS78]; see also [RSS94]. For the proof of the Birman-Schwinger bound, see [RS78]. The monograph [HS96], besides the introduction to spectral theory, contains the proofs of many results in Sections 1.1-1.2; see also the monograph [CFKS08] for these and other results.

Section 2 is based on the fundamental paper [Fad64], classical surveys [Fad59, Fad74], and the monograph [Mar86], devoted to the inverse scattering problems. For more information and details on the material in Section 2.1 and Problems 2.2, 2.3, 2.4, see [Fad64] and [Mar86]. The complex integration of the resolvent kernel is a powerful method for proving the eigenfunction expansion theorem, especially in the presence of the absolutely continuous spectrum, and in Section 2.2 we followed the elegant approach from [Fad59]; Problem 2.6 is taken from [Fad74]. Section 2.3 is based on [Fad59, Fad64, Fad74]; see also the monograph [New02] for a comprehensive exposition of the scattering theory from the physics perspective, and the recent book [Yaf92] for its abstract mathematical formulation. We refer the reader to [**Fad**74] and references therein for more details on the material in Section 2.4.

Section 3 is fairly standard; from a physics point of view, its material can be found in almost any textbook on quantum mechanics; see [LL58, Foc78] for a clear exposition. It was H . Weyl who introduced Lie groups into quantum mechanics [Wey50], and nowadays representation theory of Lie groups is a part of the theoretical physics curriculum; see, e.g., [BR86]. There are also many mathematics textbooks and monographs on representation theory of compact Lie groups; see, e.g., [Kir76, FH91], as well as [Vil68]. Section 4 contains the standard material presented in any textbook on quantum mechanics; see [LL58, Foc78, Mes99] for the physics presentation. Our goal here was precise mathematical formulation of the basic facts; for the proofs of all results in this section (and of the problems as well), and for their generalizations, we refer the reader to the treatise [RS79].

The solution of the eigenvalue problem for the hydrogen atom, given by E . Schrodinger in 1926, was the major triumph of quantum mechanics. Before that, the energy levels of the hydrogen atom were obtained by N. Bohr in 1913 using the Bohr model (later replaced by the Bohr-Sommerfeld model and the BWS quantization rules), and in 1926 by W. Pauli by using the quantum Laplace-Runge-Lenz vector. Sections 5.1 and 5.2 are standard and our exposition follows [LL58, Foc78]. We started Section 5.3 by presenting Pauli's approach (see [BR86] for more details on representation theory). The hidden SO(4) symmetry of the hydrogen atom was discovered by V.A. Fork, and the end of Section 5.3 is based on [Foc78] (see
[BI66a, BI66b] for more details and for the treatment of the absolutely continuous spectrum).

There exists an extensive literature on semi-classical asymptotics and the WKB method, which we just barely touched on in Section 6. We refer to [LL58] and [Dav76] for a physics discussion and to [GS77, BW97] for a mathematical introduction. Detailed exposition of the one-dimensional WKB method can be found in [Olv97] - a reference book on special functions used in this chapter. We refer to the monographs [MF81] and [Ler81] for the detailed exposition of the much more complicated multi-dimensional WKB method.

4. Notes and references about Integration in Functional Spaces by Takhtajayan

There is a vast literature on Wiener integration theory and Brownian motion, and here we present, in a succinct form, only the very basic facts. Material in Section 1 is standard, and our exposition follows the exercise section in [Rab95]. For necessary facts from probability theory, including Kolmogoroff's extension theorem and an introduction to the stochastic processes, we refer to the classic treatise [Lo77, Lo78] and recent text [Kho07]. In particular, the statement $\mu(\mathscr{H}) = 0$ in Proposition 1.1 follows from the strong law of large numbers.

Th elegant construction of the Wiener measure in Section 2 belongs to E. Nelson [Nel64], and our exposition, including the proof of the Feynman-Kac formula, follows [RS75]. We refer the reader to Ito-McKean's classic monograph [IM74] for the construction of the Wiener measure from the probability theory point of view; along this way Problems 2.1 and 2.2 get solutions. The classic book [Kac59]
and lectures [Kac80] by M. Kac are another excellent source of information on Wiener integration and its applications in different areas of mathematics. The relation between Wiener and Feynman path integrals in Section 2.3 belongs to E. Nelson [Nel64]. Problem 2.6 is taken from R.H. Cameron's paper [Cam63] (see also [RS75]); this result shows that there is no complex-valued analog of Wiener measure associated with the complex diffusion coefficient with $\operatorname{Re} D > 0$ (as opposed to the statement made in [GY56]).

Theorems proved in Section 3 serve as a rigorous foundation for our discussion of the Gaussian Feynman path integrals in Section 4 of Chapter 5. Our proof of Theorem 3.1 in Section 3.1, which uses the method of finite differences, follows the outline in [GY56] which attributed it to [Mon52]. The proof of Theorem 3.2 in Section 3.2 seems to be new.

The Euclidean quantum mechanics, obtained by replacing the physical time t by the Euclidean (or imaginary) time $-it$, is ultimately related to the theory of stochastic processes. It can be formulated by a set of axioms of the one-dimensional Euclidean quantum field theory, and we refer the interested reader to [Str05] for the detailed discussion.

Notes and references about supersymmetry

The goal of Section 1, besides giving a definition of a supermanifold, was to introduce the isomorphism $\mathcal{A}^\bullet(M) \simeq C^\infty(\Pi TM)$, emphasized by E. Witten [Wit82a, Wit82b], and commonly used in the physics literature. For a systematic introduction to supermanifolds, we refer to the classic texts [Kos77, Ber87], as well as to the modern sources [Man97, DM99, Var04] and references therein. A detailed exposition of equivariant cohomology and localization in the finite-dimensional case can be found in the monograph [BGV04]; our proof of the Berline-Vergne localization theorem in Section 2.1 follows [Sza00]. Our presentation of the infinitedimensional case, based on [BT95, Sza00], is at a physical level of rigor. Theorem 2.3 was originally formulated by E . Witten in his famous path integral derivation of the Atiyah-Singer formula for the index of the Dirac operator. Witten's original approach was lucidly presented by Atiyah [Ati85]. Our exposition follows [Wit99b], with special attention to constant factors; see also [AG83, Alv95], as well as [BT95, Sza00].

For a detailed explanation of the functor of points and a discussion of classical mechanics on supermanifolds, see [Fre99]; our examples of classical systems are taken from [Alv95]. Supersymmetry introduced in Sections 4.2-4.3 is called $N = \frac{1}{2}$ supersymmetry and is obtained as a reduction of $N = 1$ supersymmetry; see lectures [Alv95, DF99b, Fre99, Wit99a, Wit99b] and [CFKS08] for more details and references. In particular, [Fre99, Wit99a] describe useful superfield formalism for producing supersymmetric Lagrangians, sketched in Problem 4.3 in Section 4.3. Material in Section 5 is based on [Alv95]; we refer the reader to the monograph [BGV04] for the invariant definition of Dirac operators on spin manifolds and related topics.

It should be emphasized that our derivation of the Atiyah-Singer formula in Section 6 is

purely heuristic. Rigorous justification of this approach using Ito-Malliavin stochastic calculus was made by J.-M. Bismut [Bis84a, Bis84b, Bis85]; it turns out that formula (6.2) in Section 6 requires an extra factor: the exponential of the integral along the path of a multiple of a scalar curvature. When $T \to 0$, this rigorous formula for the index coincides with the heuristic expression (6.2). Still, the integration of a differential form of "top degree" over the loop space in [Bis85] remains formal, and is a challenging open problem. Finally, we refer the interested reader to [ASW90] for a path integral derivation of the H . Weyl character formula, and to [Wit99b] for the treatment of the Dirac operator on the loop space.

Литература по прикладной квантовой механике

[20] Шмиедт Вольфрам для квантовой механики

Хорошо объяснены решения некоторых простейших задач. Обязательно вскоре впишу, уже многое заготовлено!!! шаг по основам - и все, займусь численным решением, прога уже тоже готова к этому! Первая прикладная книга, которая будет вписана.

[21] А.Мессиа Квантовая механика.

имею в планах почитать, потому что в отличие от Ландау много общих интересных вопросов рассмотрено там, так что интересно многое из него добавить. так что после того, как создам по основным книгам - почитаю, доделаю разные параграфы.

хотя по сути это тот же квантмех, ее хочется прочитать просто, но это после того, как важное сделаю.

[22] (????)

О квантовых полях, связанная с квантовой механикой

[23] Ландау Л Д Лифшиц Е М Кватовая электродинамика

разные отдельные концепции взял, потому что квантовая механика переходит в КТП, так что эти связи также будут проработаны.

A.4.3 Additional Literature on Other Topics

Дополнительные обучающие книги, методички

Physicspages Quantum Mechanics 2021 https://physicspages.com/TOC-Quantummechanics.html

Куча методичек (или решенных задач) по разным тем, большая вероятноть, что то, что ищется, найдется. Жаль, что всё время до 2021го года не было это доступно...

[24] Sakurai J.J. Modern quantum mechanics. Addison Wesley Publishing Company, 1994

Typical good student book, very famous, covers all typical university topics. Nothing is very special about it, Zhou wrote that there are typos, but I wasn't reading it much.

Franz Schwabl Advanced Quantum Mechanics

A good book with some good computations in some topics, might be very useful for understanding some concepts. It is not the main book, because many also important topics are not there. I'll look at it and increase the level of mu sections later.

[25] Littlejohn R. Physics 221AB: Quantum Mechanics

Many excellent and pretty famous lectures that can help a lot!

(ЕК) Елютин Пт.В., Кривченков В. Д. Квантовая механика с задачами
301 страница теории и указаний на задач, наверное, крутые задачи. Потом добавлю их и теорию, пока хватает других тем на тренировку.

[26] Игошин Ф.Ф., Самарский Ю. А., Ципенюк Ю. М. Лабораторный практикум по общей физике. Квантовая физика
Прекрасный вузовский лабораторный практикум, где также коротко приведена основная теория типичных тем.

[27] Левитов Шитов Функция Грина
Очень много короткой теории и задач добавится. Важная книга, но это не совсем квантовая механика, так что не среди основных.

Е. С. Андрианов, А. П. Виноградов, А. А. Пухов ЛЕКЦИИ ПО КВАНТОВОЙ ОПТИКЕ Учебное пособие МОСКВА МФТИ 2018
Обсуждается много полезных моделей квантовой механики, думаю, точно многое из них добавлю в эту запись.

Базь А.И., Зельдович Я.Б., Переломов А.М. Рассеяние, реакции и распады в нерелятивистской квантовой механике
Очень хорошая книга, в которой отвечены очень многие вопросы, которые возникают в квантовой механике. (!!! многое выгружу потом отсюда!)

[28] Сивухин Д.В. Атомная и ядерная физика
Большая книга с введением в многие темы и подробным обсуждением. Не все темы актуальные, и всё равно, чтобы разобраться, потом придется открыть специализированную литературу. Не рекомендую читать, если нет лишнего свободного времени.

Robert G. Littlejohn Fall 2019 Notes 21 Time Reversal https://bohr.physics.berkeley.edu/classes/221/1112/notes/timerev.pdf
Небольшая методичка по обращению времени, гуглится, вроде бы в ней хорошо раскрыта эта тема. Подумаю еще раз про это потом.

Л. П. Суханов Лекции по квантовой механике МФТИ
Типичные лекции физтеха до того, как не начали пихать в программу кучу лишнего. Полезная, если хочется увидеть основные формулы или простую теорию. (!!! кстати, выпишу в 1ю часть из нее многое!)

Banks T. Quantum Mechanics: An Introduction
Большая книга на первый взгляд обычной теории. Возможно, что-то особенное есть и там, но похожа на просто обычный хороший вузовский учебник.

Нохрина Е. Е. Сложение двух моментов в квантовой механике Учебно-методическое пособие
Возможно, хорошее объяснение темы, в планах её додумать, хотя, возможно, я уже знаю всё из неё.

Е. Е. Нохрина Теорема Вигнера–Эккарта Учебно-методическое пособие
Возможно, хорошее объяснение темы, в планах её додумать. Больше математическое.

Ишмухаметов, Б. Х., Кацнельсон, М. И., Поликарпов, А. Ф. Одноэлектронные задачи квантовой механики в квазиклассическом рассмотрении. Краткий курс ВКБ Учебный электронный текстовый ресурс
Методичка по квазиклассике, 65 страниц, вроде хорошая и полезная.

El-Batanouny M. Advanced Quantum Condensed Matter Physics
Про фазу Берри скорее всего отличная теория, которая в Левене нам давалась. Многое выгружено, разберусь позже, у меня должна быть написана подготовка к этим темам, которые в физике твердого тела используются.

Andrei Tokmakoff Time Dependent Quantum Mechanics and Spectroscopy
I was reading about density matrix from this book. I don't know, if it is a good book, but at least about density matrix it has some information. Looks like there is a lot of topics which are not present in a basic course of QM at all!

Mitchel Weissbluth Atoms and Molecules
This book looks like it is a great introduction to QM with emphasis on models of atoms and molecules. It has basic theory and, maybe, many examples of applications. Maybe it is the best book to learn atoms?

George C. Schatz Mark A. Ratner Quantum Mechanics In Chemistry
Maybe this book is an excellent bride from QM to chemistry? Still, all basic questions about it would require weeks or months of learning.

Mladen Pavicic Quantum Computation and Quantum Communication: Theory and Experiments
A great mini encyclopedia about experiments in quantum information. Looks like it is essential for real understanding this part of physics. But the author is not that famous, so I am not sure that topics from it are important.

Други задачники

(МС) Мартинсов Смирнов Квантовая Физика для Баумана
Вроде неплохая методичка по основам, которые итак понятны после продумывания обычного курса.

(Ф1, Ф2) Флюгге З. "Задачи по квантовой механике (в 2 томах)", Мир, 1974
Хорошая книга с подробно разобранными небычными задачами. Просто итак очень много современных книг, где уже много задач разобрано, так что вряд ли есть смысл открывать её. Потом, когда-то, когда решено будет штук как минимум 200 задач из основных книг, можно будет и его порешать.

K.K.Prasad Quantum Chemistry Through Problems and Solutions
1/2 of book is basic QM problems, but another 1/2 - is a collection of very unique for QM problems. Maybe it is a really great book to understand these parts of QM about applications to chemistry? Otherwise like in Landau's book, the theory is written, but what is next? Here is what is next: this book.

(ККЧ) И.В. Копытин, А.С. Корнев, Т.А. Чуракова Задачи по квантовой механике ч 1, ч 2, ч 3.

Хорошая методички, немного задач решены, полезно и не сложно написано, 3 книги.

(Г-1981) В.М.Галицкий, Б. М.Карнаков, В.И.Коган Задачи по квантовой механике, 1981

Есть задачи, которых нет в сборнике 1992-го года. Так пока сложно сказать, какая версия лучше, потому что эта более компактная и содержит тоже многие отличнейшие задачи.

(БКП) В.С. Булыгин, М.Г. Кремлев, Э.В. Прут Избранные задачи студенческих олимпиад МФТИ по курсу общей физики Долгопрудный: Издательский Дом «Интеллект», 2015. - 312 с.

Доступ через lib.mipt, дальше по http://books.mipt.ru/book/301280. Крутой сборник задач, тоже прорешаю потом его, очень интересные и простые задачи, шикарное проведение времени на них.

F. Constantinescu, E. Magyari, Translated by V. V. Grecu Edited by J. A. Spiers Problems in Quantum mechanics

Обычный неплохой задачник, если прорешать Галицкого, то потребность в нем вряд ли будет.

Популярная литература и с упрощенным изложением

Это очень важные книги, ибо популярные идеи - неотъемлемая часть квантовой механики. И в популярных книгах они прекрасно описаны, так что радуемся и используем.

(пока не смотрел тут почти ничего, только после теормина мб буду прорабатывать)

[29] Каку М. Физика невозможного

Популярная интересная книга для мотивации и кругозора, однако не думаю, что всерьез использовать темы из неё кому-то придется.

[30] Каку М. Параллельные миры: Об устройстве мироздания, высших измерениях и будущем Космоса

Наверняка много интересной теории, но выглядит как популярная литература просто поболтать о заведомо неизвестном.

[31] Иванов, М. Г. Как понимать квантовую механику

Большая, философско-обзорная книга с обсуждением многих общих вопросов. Прекрасная книга на свободное время, но для минимальной подготовки она излишня.

[32] Фейнман Р. Квантовая электродинамика

Известные лекции по квантовой механике. Я пока не читал, итак хватает материала для изучения. Не знаю, что в них особенного?

[33] Мухин К. Н. Занимательная ядерная физика

Открыл, интересно, но абсолютно не актуально. В свободное время на пенсии почитать - хорошая идея.

Справочники

(некоторые уже видел, нужно будет - допишу)

[34]
Д. А. Варшалович, А. Н. Москалев, В. К. Херсонский Квантовая Теория Углового Момента Аппарат Неприводимых Тензоров Сферические Функции 3nj-символы Издательство Наука: Ленинградское Отделение Ленинград - 1975
Библия углового момента, огромная книга с кучей формул про сложение моментов.

A.4.4 Articles on Special Models, Experiments and Special Methods

Статьи про различные эффекты квантовой механики

[35] Л. А. Халфин Квантовый эффект Зенона
статья про квантовый парадокс зенона. интересно изучить, уйдет скорее всего часа 3 на нее, пока не актуально.

[36] Purcell, E. M Spontaneous Emission Probabilities at Ratio Frequencies
Атом спонтанно в резонаторе может излучать быстрее, оказывается! Я это не понимаю, это удивительно, потом подумаю про это, теорию доработаю для него.

Ales Navrat Geometric phase in quantum theory, 2006
A good review of Berry phase by a student.

Д.Н. Клышко Геометрическая Фаза Берри В Колебательных Процессах Ноябрь 1993 Г. Том 163, № 11 Успехи Физических Наук
Вроде крутая статья про фазу Берри, может, когда-то дойду до неё?

A. Tomita, R. Y. Chiao, "Observation of Berry's topological phase by use of an optical fibre", Phys. Rev. Lett. 57 (1986) 937-940.
This was the first experiment to confirm the prediction of Berry.

R.Y. Chiao and Y.S. Wu, "Manifestations of Bery's topological phase for the photon", Phys. Rev. Lett. 57 (1986) 933-936.
Realization of the first experiment to confirm the prediction of Berry.

Статьи про теоретические методы

[37] Aharonov, Yakir and Albert, David Z. and Vaidman, Lev How the result of a measurement of a component of the spin of a spin-1/2 particle can turn out to be 100
Можно измерить спин частицы равный 100, почему - тут когда-то почитаю, очень интересно.

[38] Hubac, Ivan and Wilson, Stephen Brillouin-Wigner Methods for Many-Body Systems
Крутая книга на 190 страниц про теорию возмущений, еще по приложениям в атомной физике и диаграммам Фейнамана, сделаю основы - скорее всего почитаю. После нее по идее очень хорошо теория возмущений станет понятна.

В. М. Шабаев, Теория возмущений Рэлея–Шредингера для релятивистского атома, ТМФ, 1990, том 82, номер 1, 83–89

Рассуждения про теорию возмущений. Выглядит интересно, однако не факт, что она полезная. Когда-то посмотрю, по идее с ней может стать глубже понятны теория возмущений и атомы.

[39] Sergey Bravyi and David P. DiVincenzo and Daniel Loss Schrieffer–Wolff transformation for quantum many-body systems

Оказывается, есть такие преобразования, которые в многочастичных системах применяются. Наверное, хорошая статья, выглядит как 5 дней моей работы над ней, чтобы понять. Там в многочастичных системах еще много статей и тренировок мне нужно, чтобы научиться им.

Статьи про моделирование

[40] Feldbrugge, Job and Pen, Ue-Li and Turok, Neil, Oscillatory path integrals for radio astronomy

В конце описан эксперимент Юнга и переход в классику, неплохое дополнение, потом отработаю.

https://jfeldbrugge.github.io/Schrodinger/ Job Feldbrugge Уравнение Шредингера: The Suzuki-Trotter integrator Young's double-slit experiment

численное решение УШ в математике, интересное моделирование. как сделаю основные записи - за часа 3 пойму, как это моделирование устроено. очень будет крутое дополнение.

Статьи про атомную физику и теорию к ней

https://www.chemistry.tcd.ie/assets/pdf/ss/DAMB/DAMBSS/PERTURBATIONTHEORY.pdf Rayleigh-Schrödinger Perturbation Theory

Автор неизвестен. 17 страниц про теорию возмущений в атомной физике, по идее это все уже должно быть известно, но когда-то может еще подчитаю, там скорее всего пара интересных еще есть деталей.

A.4.5 Additional Literature on Other Topics

Обсудим самые основные профессиональные книги о науках, связанных с квантовой механикой.

(ими займусь, когда основные проработаю, не раньше)

Статьи п атомной физике

Зоммерфельд А. Строение атома и спектры. Том 1

Когда-то открывал, никогда не доходил до прочтения.

Статьи по ядерной физике

Основная и вводная по статистической физике, магнетизму

[41] Nicola A. Spaldin Magnetic Materials: Fundamentals and Applications

Известная книга про простой магнетизм и введение в сложные темы.

[42] Боголюбов Н.Н., Боголюбов Н.Н. (мл.). Введение в квантовую статистическую механику Изд. 3 URSS. 2018. 384 с. ISBN 978-5-9710-4456-7.

Известная книга про квантовую механику многочастичных систем, в планах почитать её.

Основная и вводная по физике конденсированных сред

Литература про математические модификации квантовой механики

В. С. Владимиров, И. В. Волович, p-Адическая квантовая механика, Докл. АН СССР, 1988, том 302, номер 2, 320–323

Если будет интересно - как раз и почитаю, пока не знаю, как там поля чисел вообще учитываются?

A.5 Overview of Quantum Mechanics

Выделим самое главное, что есть в квантовой физике, чтобы уверенно пользоваться ей.

A.5.1 Quantum Mechanics in 2 Hours

Обсудим в двух словах всю квантовую механику.
(потом напишу, пока вообще не актуально)

Map of quantum mechanics

(add picture and discussion about it!!!)

Введение в квантовую механику для тех, кто ничего о ней не слышал

(сформулирую потом)
(найду какую-то красивую фотку потом, тут была некрасивая, удалил ее)

наглядное представление как строится квантовая механика

О методах решений уравнений квантовой механики

(тут максимально коротко, все формулы)

Появление квантовой механики в нашей картине мира

обзор типичных моделей

Обсудим, какие модели существуют?
излучение, рассеяние, теория атомов, (?)
их не много, это типичные применения квантовой механики, которыми мы и занимаемся.

Качественное отличие квантовой механики и классической

(конкретно приведу эти отличия. нпр там рассеяние такое, тут - такое. укажу, почему. пока не готов писать это.)

О точно решаемых моделях квантовой механики

(соберу их, указав суть и идею решения)
- атом водорода
- осциллятор

многие задачи на обобщенные функции:
- задача Ландау-Зенера
- куча всего (да??)

Определения квантовой механики

выпишу из теории ниже, по итогу что есть что.

Определение кванта

Квант - это
(тут пояснение, почему это определение важно, порой на самом деле про это возникают большие дискуссии)

Определение квантования

Квантование это -.....
(тут пояснение, почему это определение важно, порой на самом деле про это возникают большие дискуссии)

О границе применимости квантовой механики

какой должна быть система, чтобы к ней применялась квантовая физика?

четко пропишу. пока хз.

О типичных мысленных экспериментах в квантовой механике (?)

(потом напишу)

основы квантового описания

Классическая механика неплохо описывает при привычный нам мир.

Зная начальные данные с помощью второго закона Ньютона можно однозначно описать поведение частицы.

В квантовой физике вводится состояние системы, и решается уравнение Шредингера.

Со временем волновая функция расплывается (?)

Таким образом в классической механике и квантовой есть одно уравнение, которое описывает все происходящее в будущем.

но после измерения мы видим конкретную точку в пространстве.

возникает вопрос, как согласовать волновую функцию и измерение с конкретным значением?

Переход из волновой функции в частицы совершенно случаен, но известно, что модуль ее в квадрате дает вероятность нахождения частицы в данной точке пространства.

Это предположение было высказано Борном.

Эйнштейну это не понравилось.

Таким образом, пока мы не смотрим, существует волновая функция, а как только мы смотрим, она коллапсирует и мгновенно появляется частица.

кот Шредингера

(!! после текста будет все с формулами!!)

Шредингеру это очень не нравилось.

поэтому он придумал эксперимент с котом Шредингера.

Мы возьмем коробку, поместим в нее кота, добавляем атом радиоактивного элемента и детектор типа счетчика гейгера, который при срабатывании выпустит радиоактивный газ.

оградим от вмешательства самого кота.

если атом распадается, то детектор улавливает радиацию, испускает радиоактивный газ и кот погибает.

если не срабатывает, кот живет дальше.

состояние кота зависит от состояния детектора и атома, назовем эту связку запутанностью

разве что атому не обязательно быть распавшемся или не распавшемся, потому что согласно квантовой механике, большую часть времени он находится в суперпозиции состояний, он одновременно распавшийся и не распавшийся, пока его не измерят его.

таким образом состояние запутанное и пока мы не произведем измерения, одновременно вся коробка находится в двух состояниях, где атом распался и кот мертв, или где атом не распался и кот жив.

Тем самым Шредингер хотел сказать, что такого быть не может.

Поэтому у нас есть глава про другие объяснения квантовой механики.

(и что еще?)

суперпозиция, запутанность, измерения (??)

(откуда я эту хрень вытянул?)

Итак, у нас есть три понятия, с которыми нужно разобраться: суперпозиция, запутанность, измерения.

суперпозиция - что объект может находиться в двух состояниях одновременно.

(?) Если например в опыте Юнга описывать электрон волновой функцией, то может показаться, что электрон проходит через две щели одновременно.

запутанность - что если после взаимодействия двух частиц мы измерим одну волновую функцию - моментально сколлапсируется вторая.

то есть это как если бы была одна волновая функция на двоих частиц.

может показаться, что так как все взаимодействует со всем, то есть одна волновая функция для всей вселенной.

но и про волновую функцию отдельной частицы говорить также можно.

запутывание происходит только в момент взаимодействия с другими объектами.

то есть запутанность - что состояние двух разных частиц можно описывать одной волновой функцией.

измерения.

измерение это взаимодействие.

Типичные квантовые соотношения

В квантовой физике имеются некоторые фундаментальные формулы, которые позволяют делать ключевые переходы, а также раскрывают суть понятий.

(тут будет обсуждение, откуда взялись эти соотношения и когда они верные, когда нет)

Энергия через параметры $E = \hbar\omega$

распространяющаяся материя при взаимодействии с веществом распадается на конечный набор корпускул, энергия каждой:

$$E = \hbar\omega.$$

Энергию можно записать через длину волны как

$$E = \hbar kc = \frac{2\pi\hbar}{\lambda},$$

то есть она обратно пропорциональная длине волны.

Соотношение де Бройля $p = \hbar k$ в двух словах

Суть соотношения де Бройля в том, что

$$p = \hbar k.$$

Его можно получить из (????)
На этом моменте видно, что зная импульс, сразу мы знаем волновое число
(как вводится кстатиати оно? на теорпол все падает).
(?? в чем смысл его)
что частица есть волна мб, но тут подумать можно.

Длина волны через параметры

Длина волны через энергию выражает, расписав формулу $E = \hbar\omega$, в итоге

$$\lambda = \frac{hc}{E}$$

соотношение де Бройля: обзор применений

Часто есть задачи про него, так что соберем теорию для него

волновые характеристики любого тела

можно посчитать волновые характеристики любого тела, пока не задумываясь, что это значит. ?????

$$\lambda = \frac{2\pi}{k} = \frac{2\pi\hbar}{p} = \frac{2\pi\hbar}{m\upsilon} = \frac{2\pi\hbar}{\sqrt{2mE}}$$

Критерием, который говорит, когда частица - корпускула, а когда волна(откуда?) введена была волновая функция частицы.

Обзор формализмов квантовой механики

обзор способов описания квантовых систем

(что есть там волновая функция, а есть матрица плотности, опишу сравнение этих методов. сперва в них разберусь нормально.)

Обзор дальнейших развитий формализма

Обзор математизированной квантовой механики

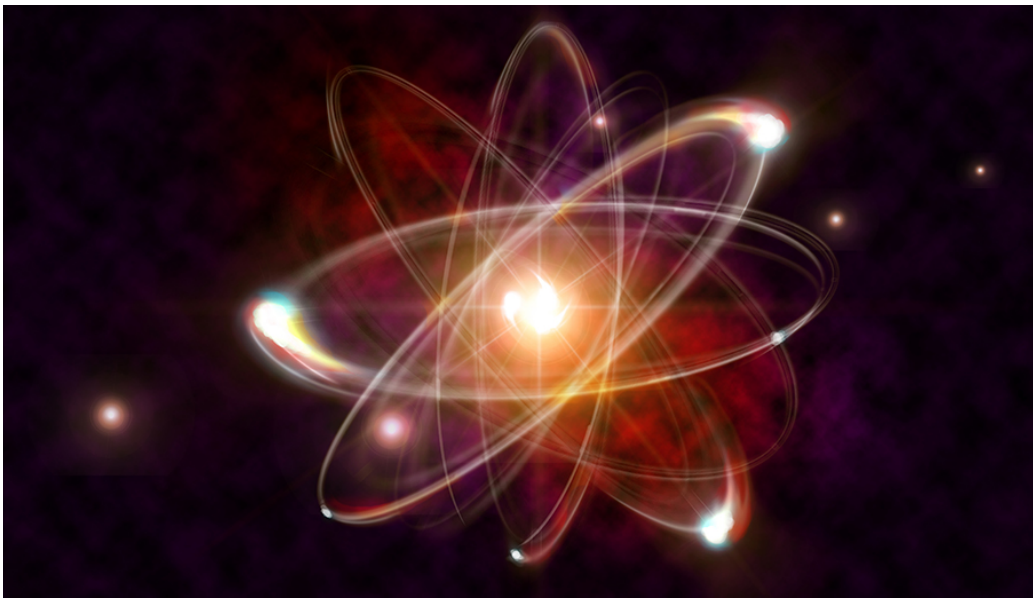
Обзор операторов в квантовой механике

(напишу, что такие-то есть, такие-то их особенности ключевые)

A.5.2 Popular About Quantum Mechanics (??)

(!!! напишу потом круто и нормально! много книг - примеры как это можно написать! мб страниц 15 потом будет, но качественной записи!)

Каков квантовый мир?



A.5.3 Overview of Sections of Quantum Mechanics

Об атомной физике

О квантовых числах

(опишу, какие есть, ориентироваться в них - базовая подготовка)

A.5.4 Seeing a Quantum World (???)

(тот самый взгляд, который я аж целой частью хотел сделать! опишу, как мы вообще видим квантовую механику, когда все изучили уже! пока все еще не готов написать)

(здесь просто обозреваем квантовый мир и смотрим на разные принципиальные его закономерности. много феноменологии и популряных тем. то, что раньше на целую часть хотел растянуть)

A.5.5 Mathematics in Quantum Mechanics

обзор применений теории групп в квантовой механике

Связь с теорией вероятностей

по сути с вероятностями работаем же?
подумаю, как связаны они?

Связь с теорией меры

Там как-то она строится через нее, вот потом и узнаю.

A.5.6 Connections with Other Parts of Physics

Для углубленного понимания подхода квантовой механики, подчеркнем её фундаментальную связь с другими разделами.

Связь с механикой

Одна из из главных связей - это связь с механикой, её обсудим первее всего. На самом деле конструкция эта широко известна и ниже она написана сполна хорошо.

Связь с оптикой

сформулирую потом ту самую связку важную.

Связь со статистической физикой

A.5.7 Overview of Typical Quantum Phenomena

Приведем группировку типичных явлений, которая позволит в них ориентироваться.
все заготовки из овчоса. прорешаю его - пропишу.

A.5.8 Quantitative Estimates

Приведем типичные масштабы квантовых величин для полной ориентации и сравнения.

(полезный очень раздел, чуть что - его и использую, пересоберу потом нормально, когда опыт появится)

например, импульс измеряется в $\frac{eV}{c}$, c - скорость света.
по порядку величины энергия электрона - несколько эВ.

Характеристики типичных объектов

Значения типичных величин

Приведем значения типичных величин.
(с опытом нормаьлно сбласнсирую)

Свойства электрона

Масса электрона
$9.1 \cdot 10^{-31}$ кг.
Типичный импульс электрона?????
радиус электрона????
Энергия электрона:

$$E_e = m_e c^2 \approx 0,51\text{МэВ}$$

10^{-13}см - размер атома.
при комнатной температуре $kT = 0,1\text{eV}$.
(?)
величина ямы потенциальлной в атоме: $4 - 5eV$
колебательная энергия на одну молекулу $\sim 0.1 \sim 10^3 K$
если $\lambda \sim 5mkm$, то $\hbar\omega \sim 0,2eV$
можно делить и умножать на $2r_b^2 m_e/\hbar$, сводим расчеты к ридбергу.
дальше $\hbar\omega$ и массы можно подставлять.

Свойства других частиц

масса протона
$m_{\text{протона}} = 1,67 \cdot 10^{-29}$ кг.

Свойства типичных атомов (!!!)

(тут подготовка по общей физике!)
радиус Бора

$$a = \frac{\hbar^2}{m_e e^2} \approx 5 \cdot 10^{-9}\text{см}$$

типичные значения волновых функций

в основном состоянии атома водорода его волновая функция - экспонента.

Константы

Часто полезно в преобразованиях приводить величины к одной из типичных констант квантовой механики. Обсудим их ниже.
(мб потом даже укажу, в каких местах какая возникать будет)

Фундаментальные константы

Постоянная Планка:
постоянная планка имеет вид:

$$\hbar = 1,054571 \times 10^{-34}\text{Дж} \cdot \text{с}. = 1,054571 \times 10^{-27}\text{эрг} \cdot \text{с}; = 6,582119 \times 10^{-16}\text{эВ}.$$

,
Также встречается

$$h = 2\pi\hbar$$

которая удобна в????
размерность совпадает с размерностью момента импульса (????)

(а смысл ее какой?)
(откуда такое значение?)
Магнетон Бора

$$\mu_{\text{B}} = \frac{e\hbar}{2mec} = 0,92740 \cdot 10^{-20}{}_{\text{e}}/\text{Гс}$$

Ядерный магнетон

$$\mu_{\text{gR}} = \frac{e\hbar}{2m_{\text{p}}c} = 0,50508 \cdot 10^{-23} \text{ эрг } /\text{Гс}$$

Постоянная тонкой структуры

$$\alpha = \frac{e^2}{\hbar c} = 7,2973 \cdot 10^{-3} = \frac{1}{137,036}$$

Постоянная Ридберга

$$R_\infty = \frac{me^4}{4\pi\hbar^3 c} = \frac{\alpha^2}{4\pi\lambda_e} = 109737,31 \text{ см}^{-1}$$

Боровский радиус

$$r_1 = \frac{\hbar^2}{me^2} = \frac{\lambda_e}{\alpha} = 0,52918 \cdot 10^{-8}\text{см}$$

Квант магнитного потока (сверхпроводящий)

$$\Phi_0^{\text{сп}} = \frac{hc}{2e} = 2,0678 \cdot 10^{-7}\text{Гс} \cdot \text{см}^2$$

Квант холловского сопротивления

$$R_0 = \frac{h}{e^2} = 25812,806377\text{Ом}$$

Постоянная Стефана-Больцмана

$$\alpha = \frac{\pi^2 k^4}{60\hbar^3 c^2} = 5,6705 \cdot 10^{-5}\frac{\text{эрг}}{\text{с} \cdot \text{см}^2 \cdot \text{К}^4} = 5,6705 \cdot 10^{-8}\frac{\text{Вт}}{\text{М}^2 \cdot \text{К}^4}$$

Постоянная в законе смещения Вина

$$b = \lambda_{\max} T = 0,2898\text{см} \cdot \text{К}$$

Элементарный заряд

$$e = 4,8032 \cdot 10^{-10} \text{ ед. СГСЭ } = 1,60218 \cdot 10^{-19} \text{ К л}$$

Электрон-вольт

$$1 \text{ В} = 1,60218 \cdot 10^{-12} \text{ эрг}$$

Температура, соответствующая 1 эВ

$$T_{\text{эВ}} = 11606 \text{ К}$$

Атомная единица массы

$$1 \text{ а. е. М. } = 1,66054 \cdot 10^{-24}\Gamma(931,494\text{М} \ni \text{В})$$

Электрон

Масса

$$m_{\text{e}} = 9,10939 \cdot 10^{-28} \text{ г}$$
$$m_{\text{e}}c^2 = 0,511 \text{ МэВ}$$

Удельный заряд:

$$\frac{e}{m_e} = -5,2728 \cdot 10^{17} \text{ ед СГСЭ } = -1,7588 \cdot 10^{11} \text{К/Г}$$

Комптоновская длина волны

$$A_{\text{e}} = \frac{\hbar}{m_{\text{e}}c} = 3,8616 \cdot 10^{-11} \text{см}; \Lambda_{\text{e}} = \frac{h}{m_{\text{e}}c} = 2,4263 \cdot 10^{-10} \text{см}$$

Классический радиус

$$r_{\text{К}\pi} = \frac{e^2}{m_{\text{e}}c^2} = 2,8179 \cdot 10^{-13} \text{см}$$

Протон

Масса

$$m_{\text{p}} = 1,6726 \cdot 10^{-24}{}_{\Gamma} = 1,007276 \text{ а. е. М.}$$
$$m_{\text{p}}c^2 = 938,272 \text{М } \ni \text{ В}$$

Отношение массы протона К массе электрона

$$\frac{m_{\text{p}}}{m_{\text{e}}} = 1836,1527$$

Удельный заряд

$$\frac{e_{\text{p}}}{m_{\text{p}}} = 2,8716 \cdot 10^{14} \text{ ед. СГСЭ } = 9,5788 \cdot 10^{7} \text{ К}\pi/$$

Комптоновская длина волны

$$\lambda\!\!\!^{-}_{\text{p}} = \frac{\hbar}{m_{\text{p}}c} = 2,103 \cdot 10^{-14} \text{см}; \quad \Lambda_{\text{p}} = \frac{h}{m_{\text{p}}c} = 1,3214 \cdot 10^{-13} \text{см}$$

Магнитный момент

$$\mu_p = 2,7928 \cdot \mu_{\text{яд}} = 1,4106 \cdot 10^{-23} \text{ эрг /Гс}$$

Нейтрон

Масса

$$m_{\text{n}} = 1,6746 \cdot 10^{-24} \Gamma = 1,00866 \text{ а. е. М.}$$
$$m_{\text{n}}c^2 = 939,565 MB \text{ В}$$

Отношение массы нейтрона к массе протона

$$\frac{m_{\text{n}}}{m_{\text{p}}} = 1,001378$$

Комптоновская длина волны

$$\lambda\!\!\!^{-}_{n} = \frac{\hbar}{m_n c} = 0,210 \cdot 10^{-13} \text{см}; \quad \Lambda_n = \frac{h}{m_n c} = 1,31959 \cdot 10^{-13} \text{см}$$

Магнитный момент

$$\mu_n = -1,9130 \cdot \mu_{\text{яд}} = -0,9662 \cdot 10^{-23} \text{ эрг /ГС}$$

Типичные составные константы

(вот именно их чаще всего мы используем в быстрых преобразованиях!)
постоянная Ридберга 109722,267 $\frac{\text{эрг}}{\text{см}^2} = 10^5 \frac{\text{дин}}{\text{см}}$

$$R_g = \frac{\hbar^2}{2m_e r_b^2} = \frac{l^2}{2r_b} = 13,6eV \tag{A.1}$$

$r_b = \frac{\hbar^2}{m_e e^2}$ - радиус бора!
постоянная тонкой структуры!!! $\frac{e^2}{\hbar c} = \alpha$
постоянная тонкой структуры:
магнетон бора:
$\mu_B = \frac{e\hbar}{2cm_e}$

комптоновская длина волны

Разберём все, что с ней связано, там полно деталей интересных.

g-фактор

тоже популярная конструкция.

единицы измерения СГС

Приведем все необходимые знания про СГС

см, г, с,...

Энергия в СГС

про энергию:
1 eV = 1,6 10^{-19} Дж.
1 eV = 11600 K
Энергия в эВ через длину волны может быстро быть численно посчитана:

$$E = \frac{2\pi\hbar}{\lambda} = \frac{12390}{\lambda[\text{A}]}\text{эВ} \tag{A.2}$$

1 эрг = 1 гсм$^2/c^2 = 10^{-7}$Дж = $6.24150965(16) \cdot 10^{11}$ эВ = 0,6 ТэВ.

Переход в эВ

Из Джоулей чтобы перейти, просто делим на 1.6 10^{-12}

Обзор применений СГС

когда она нужна?

Атомные единицы массы

другое название Дальтон.

$$1\text{aem} = \frac{1}{12}M_{_6{}^{12}C} \cong 931,5\text{МэВ} \to 1,66 \cdot 10^{-24} \text{ г.}$$

Величины ядерной физики

Беккерель - распад в секунду.

Натуральная система единиц

единицы измерения $\hbar = c = 1$

Обсудим эту систему единиц и все нюансы, потому что как в теоретических вычислениях, так и в разных приложениях именно она используется.

Обзор применений натуральной системы

когда она нужна?
вроде когда не хочется думать про константы.
хз когда

A.5.9 Description of Notation

Структура по квантовой физике - одна из самых принципиально замороченных и непростых, и мало кто её со всех сторон в принципе собирал. Поэтому опишем, что из себя представляет эта запись, ведь именно на этой структуре и держится абсолютно всё понимание.

части записи

(потом напишу, что такая-то глава содержит такие-то темы.)

О первой части про квантовую механику в двух словах

Все, что наиболее используемое.

О первой части с основами квантовой механики

Темы теормина и указания их углублений.

О третьей части с задачами

Важнейшая часть, ради которых и сделаны другие части.

приложения

какие вообще приложения я разбирал?

A.5.10 On the History of the Development of Quantum Mechanics

(потом напишу, пока не актуально, вообще тут много разного интересного рассказать можно.)

О развитии взглядов на квантовые системы (???)

Обсудим основные моменты развития квантовой механики.
(тут много вопросов и мне не до них, на них правильнее забить пока что.)

древние подходов к квантовой механике

(!! укажу потом их пользу!!!)
там куча бреда, который не так интересен

первые квантовые теории

хз

Шредингер, Дирак,...

короче, потом мб разберу.

постулаты Бора

постулаты Бора: польза в настоящее время

они вообще нужны или как?

Об открытии таблицы Менделеева (???)

(мб напишу, есть инфа про это, но не до этого. там Мендеев что-то думал, Бор что-то думал, сейчас это супер малоприоритетно, все это поудалял, потом может быть как-то напишу без воды. а может и не напишу, будет оставленный вопрос, о чем я и не сожалею ни капли. плюс тут химию нужно помнить или знать, я на нее же забил полностью.)

Об тупиках в создании и понимании квантовой механики

(с этой стороны посмотрю на историю.)

Об истории ядерной физики

(думаю, это вообще не нужно, так, на самом деле.)

краткая история ядерной физики

резерфорд создавал свои атомы, заметил, что 1/8000 частиц летит назад.
подумав над этом он пришел к модели решения задачи на кулоновском потенциале.
все было механическое описание
резерфорд поставил перед мозли задачу, что определяет длину характеристического рентгеновского излучения?
характеристического рентгеновского излучение - это когда переход между двумя дискретными состояними определяется напрямую структурой.
и это четко выделенные пики, которые с помощью фотопластинки замечаются.
мозли показал, что закон такой-то...
азотная катастрофа.
паули был учеником кронекера.
удвоение спектра можно объяснить тем, что у электрона мог бы быть собственный магнитный момент.
черзе год...
подумали.
прибежали к эренфесту со словами отдавать назад, но ее уже послали.

в письме паули написал, что избавитсяот азотной катострофы можно, если допустить, что в ядре есть кроме протона и электрона есть нейтральные частицы с полуцелым спином. и также они при бетта распаде могут вылетать.

и так паули объяснил азотную катастрофу и непрерывный спектр бетта распада.

ситуация висела до 1932г когда чадвик нашел нейтральный протон - нейтрон.

потом Гоепперт-Майер и Енсен написали про оболочечную модель со спин-орбтальным взаимодействимем

потом производили эксперименты по кулоновскому возбуждению ядер при рассеинии альфа-частиц.

гигантский дипольный резонанс связан с огромным числом колебательных возбуждений.

и там огибающая есть, которая так и называется.

и одночастичные возбуждения есть, но они не часто наблюдаются.

они относятся к коллекстивным возбужедниям.

в 1972 году открыли гигантский квадрупольный резонанс.

дипольный - значит был передан дипольный орбитальный момент, квадрупольный - значит передается орбитальный момент =2, монопольный =0.

1949 M. Goeppert-Mayer, D. Jensen: Оболочечная модель со спин-орбитальным взаимодействием

1950− Эксперименты по кулоновскому возбуждению ядер при рассеянии $\alpha-$
1953 частиц. - ротационные, $E_I \sim \frac{I(I+1)}{2\mathcal{J}}$(десятки k ∋ B)
- колебательные, $E_k \sim \hbar\omega \cdot k$ (M_3B)
- Одночастичные,)несколько M_3B) A. Bohr, B. Mottelson, J. Rainwater
1972 Открытие гигантского квадрупольного резонанса в (e, e') и адронных реакциях
1977 Открытие гигантского монопольного резонанса
1961 Открытие изобар-аналогового резонанса в (p, n)
1979 Открытие гигантского гамов-теллеровского резонанса в (p, n)

он идет благодаря взаимодействим спинов.

происходит в бетта распадах.

также открывались двойные гигантские резонансы.

A.6 Puzzles for Various Occasions

Одна из главных польз квантовой механики в том, что она дает ответы на самые идейно непонятные задачи. Поэтому сразу же после появления общего представления, перейдем к обсуждению самых типичных загадок и тупиков.

A.6.1 Interesting Questions of General QM Just for Fun

(кв теор информ, формализм, математика для квантмеха, то, что интереснее всего. чаще всего именно это используется)

A.6.2 Interesting Questions of Atomic, Nuclear Physics Just for Fun

Про атомы можно задавать много идейных и очень простых вопросов, которые здесь и приведем.

момент количества движения электрона в атоме может любым.

сколько может привнести фотон - сколько угодно.

ЛЛ-140.1 Поляризация фермиона при рассеянии

Для рассеяния частиц со спином 1/2 на частицах со спином 0 определить поляризацию после рассеяния, если до рассеяния она тоже была отлична от нуля.

(в теории об этом будет, тут укажу суть этой идеи)

почему таблица менделеева такая

говорят, бор объяснил это.

я пока не уверен в формулировке вопроса

из чего состоит ядро и почему?

почему альфа распад происходит?

A.6.3 Questions for Those Who Claim They Know QM

Что такое квантование?

(почитаю Тахтаджаяна, пойму, буду спрашивать. пока не понял, почему именно так мы определяем это.)

A.6.4 Conceptual Questions on Quantum Mechanics

зависимость вероятности от частоты измерения

Будет ли уменьшаться вероятность распада нестабильного состояния, если достаточно часто измерять — распадается ли это состояние?

Будет ли уменьшаться вероятность перехода из начального состояния под влиянием фиксированного взаимодействия, если достаточно часто измерять, произошел ли этот переход?

Квантовая теория утверждает: да, что с классической точки зрения кажется невозможным и парадоксальным.

см квантовый парадокс Зенона

связь квантовой механики и энтропии

(?? чет придумал, да не знаю особо)

случайность с точки зрения квантовой механики

интересно

Что будет, если увеличить постоянную Планка?

(подробно напишу, как изменится все важное. про опыт Юнга уже знаю, но про остальное четко сказать пока не могу. мб с формулами отвечу про это)

Записать уравнение Шредингера в искривленном пространстве или в бескоординатном виде?

(мб Тахтаджаян в помощь.)

A.6.5 Fun Technical Puzzles

Тут я укажу типичные хорошие задачи по квантовой механике на тренировку типичных уравнений.

Получить релятивистские поправки к атому водорода (????)

(тут тренироваться еще нужно денёк.)

Требуется вывести формулу

$$\hat{H} = \frac{p^2}{2m} + e\Phi - \frac{\boldsymbol{p}^4}{8m^3c^2} + \frac{e\hbar}{2m^2c^2}\frac{\Phi'(r)}{r}(\boldsymbol{s}\cdot\boldsymbol{L}) + \frac{e\hbar^2}{8m^2c^2}\triangle\Phi$$

Для этого нужно знать, как работать с уравнением Дирака $(\mathcal{P} - mc)\psi = 0$, где $\mathcal{P}_\mu = \mathrm{i}\hbar\partial_\mu - \frac{e}{c}\mathcal{A}_\mu$, подставить $\psi(t,\boldsymbol{r}) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}mc^2t}\begin{pmatrix}\varphi(t,\boldsymbol{r})\\ \chi(t,\boldsymbol{r})\end{pmatrix}$ (???? тут пока проблемы), получить, что

$$\chi = \frac{1}{1+\frac{\hat{\epsilon}-e\Phi}{2mc^2}}\frac{(\boldsymbol{\sigma}\cdot\mathcal{P})}{2mc}\varphi \approx \frac{(\boldsymbol{\sigma}\cdot\mathcal{P})}{2mc}\varphi.$$

Дальше сперва найти только лишь нерелятивистское действие через верхнюю компоненту, для этого использовать некоторые формулы векторного анализа:

$$\begin{aligned} S_{\mathrm{NR}} &= \int \mathrm{d}^4x\bar{\psi}(x)(\not{p} - mc)\psi(x) = \int \mathrm{d}t\mathrm{d}^3r\varphi^\dagger\left\{\hat{\epsilon} - e\Phi - \frac{1}{2m}(\boldsymbol{\sigma}\cdot\boldsymbol{P})^2\right\}\varphi \\ &= \int \mathrm{d}t\int \mathrm{d}^3r\varphi^\dagger\left\{\hat{\epsilon} - e\Phi - \frac{\mathcal{P}^2}{2m} + \frac{e\hbar}{2mc}(\boldsymbol{\sigma}\cdot\boldsymbol{\mathcal{H}})\right\}\varphi. \end{aligned}$$

Если подставить в действие первую поправку и преобразовать с помощью векторного анализа и свойств σ-матриц:

$$\begin{aligned} S &\approx \int \mathrm{d}t\int \mathrm{d}^3r\varphi^\dagger\left\{\hat{\epsilon} - e\Phi - \frac{\boldsymbol{p}^2}{2m} + \frac{1}{4m^2c^2}(\boldsymbol{\sigma}\cdot\boldsymbol{p})(\hat{\epsilon}-e\Phi)(\boldsymbol{\sigma}\cdot\boldsymbol{p})\right\}\varphi \\ &\approx \int \mathrm{d}t\int \mathrm{d}^3r\varphi^\dagger\left\{\hat{\epsilon}\left(1+\frac{\boldsymbol{p}^2}{4m^2c^2}\right) - e\Phi - \frac{\boldsymbol{p}^2}{2m} - \frac{e}{4m^2c^2}\left(\Phi\boldsymbol{p}^2 - \mathrm{i}\hbar\{\boldsymbol{\nabla}\Phi\cdot\boldsymbol{p} + \mathrm{i}\boldsymbol{\sigma}\cdot(\boldsymbol{\nabla}\Phi\times\boldsymbol{p})\}\right)\right\}\varphi \\ &\approx \int \mathrm{d}t\int \mathrm{d}^3r\varphi^\dagger_{\mathrm{NR}}\left\{\hat{\epsilon} - e\Phi - \frac{\boldsymbol{p}^2}{2m} + \frac{\boldsymbol{p}^4}{8m^3c^2} - \frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\boldsymbol{\nabla}\Phi\times\boldsymbol{p}) - \frac{e\hbar^2}{8m^2c^2}\triangle\Phi\right\}\varphi_{\mathrm{NR}}, \end{aligned}$$

где введен φ_{NR} такой, что $\varphi = \left\{1 - \frac{\boldsymbol{p}^2}{8m^2c^2}\right\}\varphi_{\mathrm{NR}}$ и $\boldsymbol{L} = (\boldsymbol{r}\times\boldsymbol{p})$. (??? тут математика, к которой мне еще нужно тренироваться!)

Можно записать проще, явно подставив $\Phi = -\frac{e}{r}$, $\Phi'(r) = \frac{e}{r^2}$, $\triangle\Phi(r) = 4\pi e\delta(\boldsymbol{r})$, в итоге

$$V = -\frac{\boldsymbol{p}^4}{8m^3c^2} + \frac{e^2\hbar}{2m^2c^2}\frac{1}{r^3}(\boldsymbol{s}\cdot\boldsymbol{L}) + \frac{e^2\hbar^2}{2m^2c^2}\pi\delta(\boldsymbol{r}).$$

Это типичная задача на релятивистскую квантовую механику, в первую очередь для нее мы и занимались этой теорией.

Определить уровни энергии атома водорода с учетом тонкой структуры

Ответ - известная формула Зоммерфельда

$$E_{nj} = -\frac{Z^2}{2n^2}\left(\frac{e^2}{a}\right)\left\{1 + \frac{Z^2\alpha^2}{n^2}\left[\frac{n}{j+1/2} - \frac{3}{4}\right]\right\}.$$

(у белоусова порешаю еще!)

Это типичная задача по атомной физике, общефизники на нее ссылаются в книгах (? мб и в задачах). Чтобы вывести ее, нужно владеть техникой атомной физики.

вывести g-фактор электрона, а потом и поправку к нему

дано: (???)

...

Подвох задачи в том, что если к ней фигово подходить, то можно кучу раз это делать и прийти к выводу, что не способен учить квантовую физику. Такая типичная, принципиальная задача квантовой механики.

(тут будет вкратце решение, я просто всё еще тупой пока что)

B Some Mathematics and Physics for QM

Обсудим математические методы, применяемые в квантовой механике.

B.1 Some Mathematical Background

B.1.1 Elements of Functional Analysis

(какое-то введение)

про скалярное произведение скажем пару слов и методы интегрирования обсудим, дальше часто ими будем мы пользоваться.

обзор применений в квантовой физике

гильбертово пространство

свойства:

$$\langle\chi|\psi\rangle = \langle\psi|\chi\rangle^*, \quad \langle\psi|\psi\rangle \geq 0, \quad \langle\psi|\psi\rangle = 0 \leftrightarrow |\psi\rangle = 0$$

любой элемент разложим по базису.

дальше поговрим о проекторе и полноте базиса

$$|\Psi\rangle \xrightarrow{P_n} |\Psi_n\rangle$$

свойства:

$$P_n\,|\Psi_n\rangle = |\Psi_n\rangle \leftrightarrow P_n^2|\Psi\rangle = P_n|\Psi\rangle, \forall|\Psi\rangle \leftrightarrow P_n^2 = P_n$$

и у нас есть очень важный математический инструмент: разложение единицы

$$\hat{1} = \sum_n P_n = \sum_n |n\rangle\langle n|$$

дельта функция

понятно, что это такое, докажем про нее некоторые свойства.

нпр скачок производной.

а также нормировку ее.

это все нужно в задачах

Отнормируйте на дельта-функцию от энергии состояния непрерывного спектра, инфинитные в обе стороны для случая, когда потенциал растет от 0 к константе.

мы знаем свойства:

$$\int\limits_{-\infty}^{\infty} e^{-i(k-k')x}dx = 2\pi\delta\left(k-k'\right)$$

они нам понадобятся для нормировок непрерывного спектра.
она часто возникает при подсчетах интеграла и есть многие свойства интегралов с ней.
тут приведем эти свойства.

B.1.2 Useful Methods of Differential Equations for QM

Laplace Method

Обсудим метод Лапласа решения дифференциальных уравнений.

B.1.3 Special Functions for Quantum Mechanics

(see note on special functions for now, I'll collect statements from it later)

Функции Бесселя $J_m(z), Y_m(z), H_m^{(1,2)}(z), I_m(z), K_m(z)$

(тут все что нужно о них будет)
(!!! применения потом укажу, пока это не раскрыто и это очень плохо)

краткая теория функций Бесселя

Функции Бесселя являются решением диффура (какого? одного?)
И их можно понимать в аналогии с одномерным движением

$1d:$	e^x	e^{-x}	$\cos x$	$\sin x$	e^{ix}	e^{-ix}
$2d:$	$I_m(x)$	$K_m(x)$	$J_m(x)$	$Y_m(x)$	$H_m^{(1)}(x)$	$H_m^{(2)}(x)$

(?? и??? пока не так глубоко въезжаю в это)

определение и свойства Бесселей

(тут мб перепишу с методичками конста, все-таки нужна нормальная теория.
но вообще в матфизе настоящая сборка этого, тут все вкратце)

Функции Инфельда и Макдональда $I_m(z), K_m(z)$

Функции Инфельда и Макдональда являются решением уравнения

$$\psi''(z) + \frac{1}{z}\psi'(z) - \left(1 + \frac{m^2}{z^2}\right)\psi(z) = 0,$$

то есть

$$\psi(z) = A_1 I_m(z) + A_2 K_m(z)$$

Асимптотики при больших значениях аргумента:

$$I_m(z) \approx \frac{1}{\sqrt{2\pi z}}e^z, \quad K_m(z) \approx \sqrt{\frac{\pi}{2z}}e^{-z}, \quad z \gg 1$$

и при малых:

$$I_m(z) \approx \frac{1}{m!}\left(\frac{z}{2}\right)^m, \quad K_m(z) \approx \begin{cases} \frac{(m-1)!}{2}\left(\frac{2}{z}\right)^m, & m \neq 0 \\ \ln\frac{2}{z} - \gamma, & m = 0 \end{cases}, \quad z \ll 1\,,$$

где $\gamma \approx 0.577$ -постоянная Эйлера-Маскерони.

Функция $K_m(z)$ расходится в нуле. Действительно, одно из решений должно так себя вести поскольку вронскиан этого уравнения по формуле Лиувилля-Остроградского с точностью до произвольной постоянной равен 1/x.

(можно подробнее про них и их вид написать)

Функции Бесселя, Неймана Y_m, Ганкеля $H_m^{(1)}, H_m^{(2)}$

функциями Бесселя $J_m(z)$ и Неймана Y_m, либо функциями Ганкеля $H_m^{(1)}, H_m^{(2)}$ являются решением уравнения

$$\psi''(z) + \frac{1}{z}\psi'(z) + \left(1 - \frac{m^2}{z^2}\right)\psi(z) = 0$$

то есть

$$\psi(z) = B_1 J_m(z) + B_2 Y_m(z) = C_1 H_m^{(1)}(z) + C_2 H_m^{(2)}(z)$$

Функции Бесселя и Неймана имеют асимптотики при больших z:

$$J_m(z) \approx \sqrt{\frac{2}{\pi z}}\cos\left(z - \frac{m\pi}{2} - \frac{\pi}{4}\right), \quad Y_m(x) \approx \sqrt{\frac{2}{\pi z}}\sin\left(z - \frac{m\pi}{2} - \frac{\pi}{4}\right), \quad z \gg 1$$

при малых:

$$J_m(z) \approx \frac{1}{m!}\left(\frac{z}{2}\right)^m, \quad Y_m(z) \approx \begin{cases} -\frac{(m-1)!}{\pi}\left(\frac{2}{z}\right)^m, & m \neq 0 \\ -\frac{2}{\pi}\left(\ln\frac{2}{z} - \gamma\right), & m = 0 \end{cases}, \quad x \ll 1$$

И функции Ганкеля определяются как $H_m^{(1,2)}(x) = J_m(x) \pm iY_m(x)$.

Они обе, естественно, сингулярны в нуле, но представляет интерес их асимптотика на бесконечности она соответствует сходящейся и расходящейся цилиндрическим волнам:

$$H_m^{(1,2)}(z) \approx \sqrt{\frac{2}{\pi z}} e^{\pm i(z - m\pi/2 - \pi/4)}, z \gg 1$$

$$H_m^{(1,2)}(z) \approx \begin{cases} \mp i\frac{(m-1)!}{\pi}\left(\frac{2}{z}\right)^m, m \neq 0 \\ \mp\frac{2i}{\pi}\left(\ln\frac{2}{z} - \gamma\right) + 1, m = 0 \end{cases} \quad z \ll 1$$

Переход от одной функции Бесселя к другой

между функциями Бесселя имеются соотношения

$$K_m(x) = \frac{\pi}{2} i^{m+1} H_m^{(1)}(ix) = \frac{\pi}{2}(-i)^{m+1} H_m^{(2)}(-ix),$$

$$J_m(ix) = i^m I_m(x)$$

Функция Эйри

О применениях

Функция Эйри возникает буквально при решении уравнения Шрёдингера под действием постоянной силы (в постоянном электрическом поле) - потенциал $U(x) = Fx$:

$$-\frac{\hbar^2}{2m}\psi''(x) + Fx\psi(x) = E\psi(x)$$

Первым делом, как и раньше, стоит это уравнение обезразмерить.

Обратим внимание, что от энергии E можно тривиально избавиться, сделав дополнительную сдвижку начала координат:

$$z = \frac{x - E/F}{(\hbar^2/2mF)^{1/3}}$$

Такая подстановка приводит уравнение к уравнению Эйри:

$$\psi''(z) - z\psi(z) = 0$$

Его общее решение - произвольная линейная комбинация функций Эйри первого и второго рода:

$$\psi(z) = C_1\,\mathrm{Ai}(z) + C_2\,\mathrm{Bi}(z)$$

Следуя общей логике, в классически разрешённой области решения - растущие и затухающие экспоненты.

Для квантовой механики наиболее интересно решение с затухающей асимптотикой - собственно, функция Эйри - которая обладает следующей асимптотикой:

$\mathrm{Ai}(z) \approx \begin{cases} \frac{1}{2\sqrt{\pi}}\frac{1}{z^{1/4}}\exp\left(-\frac{2}{3}z^{3/2}\right), & z \to +\infty \\ \frac{1}{\sqrt{\pi}}\frac{1}{(-z)^{1/4}}\sin\left(\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right), & z \to -\infty \end{cases}$ Второе линейно независимое решение выбирается из условия, чтобы на $-\infty$ его асимптотика соответствовала косинусу; при этом, разумеется, на $+\infty$ решение - растущая экспонента [8]:

Функция Эйри возникает естественным образом при выводе граничных условий для квазиклассического приближения (мы обсудим это в соответствующем семинаре).

свойства и явление Стокса

(из птф)

Ремарка о комплексной плоскости Имеется несколько тонкостей, связанных с поведением функции Эйри в комплексной плоскости $z \in \mathbb{C}$. Более подробно эти тонкости будут обсуждаться в следуюпих семинарах, а пока просто наметим, в чём они заключаются.

Кажется естественным, что асимптотические выражения можно аналитически продолжать за пределы вещественной оси.

Однако, обратите внимание на то, что асимптотики не представляются однозначными функциями на комплексной плоскости - для их определения требуется проведение разрезов и выделение ветвей.

В то же время сама функция Эйри, разумеется, является однозначной.

Другой такой тонкостью является то, что, например, функция $\mathrm{Ai}(z)$ на $+\infty$ содержит одну экспоненту, а на $-\infty$ -две (в составе синуса), и одно из другого получить аналитическим продолжением невозможно.

Всё это связано с так называемым явлением Стокса.

В действительности, асимптотики работают только в определённых секторах комплексной плоскости, разделённых лучами (они называются линиями Стокса), на которых коэффициенты перед компонентами асимптотики (одна компонента содержит $\exp\left(\frac{2}{3}y^{3/2}\right)$, другая $-\exp\left(-\frac{2}{3}y^{3/2}\right)$) меняются скачком.

На этих линиях выражение в экспоненте является вещественным, так что одна из экспонент является максимально убывающей, а другая - максимально растущей.

За этими наблюдениями стоит интересная разработанная наука, с который некоторые из вас ещё столкнутся в процессе обучения.

комплексный метод перевала

гипергеометрическая функция

Определение

Гипергеометрическая функция в общем случае определяется от p и q параметров и имеет вид:

$$ {}_pF_q\left(a_1,...,a_p;b_1,...,b_q;z\right) = 1+\frac{a_1...a_p}{b_1...b_q}z+\frac{a_1\left(a_1+1\right)a_2\left(a_2+1\right)...a_p\left(a_p+1\right)}{b_1\left(b_1+1\right)b_2\left(b_2+1\right)\cdots b_q\left(b_q+1\right)}\frac{z^2}{2}+\cdots = $$
$$ =\sum_{n=0}^{\infty}\frac{\left(a_1\right)^{(n)}...\left(a_p\right)^{(n)}}{\left(b_1\right)^{(n)}...\left(b_p\right)^{(n)}}\frac{z^n}{n!} $$

Частные важные случаи это ${}_2F_1$ и ${}_1F_1$

Функция ${}_2F_1(a,b;c;z)$

Поговорим про ${}_2F_1$.

Альтернативно её можно определить как регулярное в нуле решение следующего дифференциального уравнения:

$$ z(1-z)f''(z)+(c-(a+b+1)z)f'(z)-abf(z)=0, \quad f(0)=1 $$

Общее решение этого уравнения имеет вид:

(место убедиться в эквивалентности определений)

Можно убедиться, что второе линейно-независимое решение этого уравнения тоже можно выразить через гипергеометрическую функцию.

Общее решение имеет следующий вид (при $c\neq 1$)

$$ f(z)=C_1{}_2F_1(a,b;c;z)+C_2z^{1-c}{}_2F_1(b-c+1,a-c+1;2-c;z) $$

К уравнению такого вида можно свести очень большой класс дифференциальных уравнений.

В действительности, имеется классификация линейных дифференциальных уравнений с дробно-рациональными коэффициентами по их особенностям в комплексной плоскости (особенностями уравнения, записанного в канонической форме $f^{(n)}(z)+p_1(z)f^{(n-1)}(z)+\cdots+p_n(z)f(z)=0$, называются особенности функций $p_k(z)$ -точки, где она обрапается в бесконечность) -в частности, у гипергеометрической функции их ровно три: $z=\{0,1,\infty\}$; и более или менее любое уравнение с тремя особенностями можно свести к гипергеометрическому виду.

Продолжая обсуждение свойств этой функции, отметим, что она не определена при целых отрицательных c (знаменатель зануляется).

Радиус сходимости ряда равен единице, и в действительности у гипергеометрической функции в точке $z = 1$ имеется особенность.

Единственное исключение из этого правила - это когда либо a, либо b - отрицательное целое число: в таком случае, ряд обраывается и превращается в полином конечной степени, имеющий, естественно, бесконечный радиус сходимости.

Последнее замечание будет важно при поиске связанных состояний.

Некоторые свойства гипергеометрической функции

(пишу только то, что применялось в квантовой механике!!! так-то много свойств разных.)

$$ {}_2F_1(a,b;c;z) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} {}_2F_1(a,b,a+b+1-c,1-z) + \\ + \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}(1-z)^{c-a-b} {}_2F_1(c-a,c-b;c+1-a-b;1-z) $$

Функция ${}_1F_1(a;b;z)$

На прошлом семинаре обсуждался обший класс гипергеометрических функций ${}_pF_q$;

однако для приложений наиболее часто встречаются именно функции ${}_2F_1$ (обсуждённая на прошлом семинаре) и ${}_1F_1$. Она, естественно, тоже определяется через гипергеометрический ряд [5]:

$$ {}_1F_1(a;b;z) = 1 + \frac{a}{b}z + \frac{a(a+1)}{b(b+1)}\frac{z^2}{2} + \cdots = \sum_{n=0}^{\infty} \frac{a^{(n)}}{b^{(n)}}\frac{z^n}{n!} $$

Кроме того, альтернативное её определение - через решение дифференциального уравнения следуюпего вида:

$$ zf''(z) + (b-z)f'(z) - af(z) = 0, \quad f(0) = 1 $$

тоже выражается через гипергеометрическую функцию [6] : $f^{(2)}(z) = z^{1-b} {}_1F_1(a-b+1;2-b;z)$. Как и с обычной гипергеометрической функцией, несложно видеть, что при целых отрицательных $b = -n$ функция не определена, а при целых отрицательных $a = -n$ она является конечным полиномом степени n. В обшем случае, отношение соседних коэффициентов разложения в ряд ведёт себя как $1/n$, поэтому радиус сходимости этого ряда - бесконечность (в отличии ${}_2F_1$, где радиус сходимости был единичным).

Асимптотическое поведение на бесконечности следуюпее:

$$ {}_1F_1(a;b;z) \approx \frac{\Gamma(b)}{\Gamma(a)} z^{a-b} e^z, \quad z \gg 1 $$

Опять-таки, мы ранее говорили, что всякое уравнение с тремя особенностями сводится к гипергеометрическому виду так и всякое уравнение с коэффициентами, которые представляют собой линейные функции z приводится к Вырожденному гипергеометрическому виду.

B.1.4 Properties of Operators in Quantum Mechanics

одно из важнейших понятий - собственный вектор.
(место про него всей записи)
дисперсия оператора вводится.

$$(\Delta F)^2 \stackrel{\text{def}}{=} \left\langle \Psi \left| (\hat{F} - \bar{F})^2 \right| \Psi \right\rangle, \quad \bar{F} = \langle \Psi | \hat{F} | \Psi \rangle$$

вообще хз, откуда мы достали это.
среднее как-то считается.
а еще собственные числа через матрицу грамма находсятся

коммутационные соотношения

важная модель и есть много на нее задач.
из этого можно даже соотношение неопределенности высрать

$$\Delta A \Delta B \geqslant \frac{\hbar}{2} |\langle C \rangle|$$

(дальше ссылка на соотношение неопределенности, у Киселева это вообще источник его.
а я хз.
просто пока что тут будет расписана его теория)

Операторные тождества

(тут порешаю потом задачи на них)

Тождества с коммутатором

$$[AB, C] = ABC - CAB = ABC - ACB + ACB - CAB = A[B, C] + [A, C]B$$

коммутаторы

Наберем математические методы, которые далее используются часто (для чего?)
Известно соотношение на коммутаторы:

$$[\widehat{\mathrm{A}\mathrm{B}}, \widehat{\mathrm{C}}] = \widehat{\mathrm{A}}[\widehat{\mathrm{B}}, \widehat{\mathrm{C}}] + |\widehat{\mathrm{A}}, \widehat{\mathrm{C}}|\widehat{\mathrm{B}}$$
$$|\widehat{\mathrm{A}}, \widehat{\mathrm{B}\mathrm{C}}| = \widehat{\mathrm{B}}|\widehat{\mathrm{A}}, \widehat{\mathrm{C}}| + [\widehat{\mathrm{A}}, \widehat{\mathrm{B}}]\widehat{\mathrm{C}}$$

Применения тождеств с коммутаторами

(тут их укажу)

$$\left[\frac{\partial}{\partial x}, x\right]$$

делаем как-то так

$$\left(\frac{\partial}{\partial x} x - x \frac{\partial}{\partial x}\right) \Psi = \frac{\partial}{\partial x}(x\Psi) - x\frac{\partial \Psi}{\partial x} = \Psi + x\frac{\partial \Psi}{\partial x} - x\frac{\partial \Psi}{\partial x} = \Psi$$

другие еще пространства и их свойства

проектор

На языке операторов то, что мы представляем, записывается так:

$$|\Psi\rangle \xrightarrow{P_n} |\Psi_n\rangle$$

$$P_n = |n\rangle\langle n|$$

$$\mathbb{1} = \sum_n P_n = \sum_n |n\rangle\langle n|$$

преобразование операторов

подробно вся та же теория операторов.
преобразовываются они так:

$$\hat{A}' |\psi'\rangle = \hat{U}_s \hat{A} |\psi\rangle = \hat{U}_s \hat{A} \hat{U}_s^\dagger |\psi'\rangle \quad \hat{A}' = \hat{U}_s \hat{A} \hat{U}_s^\dagger$$

унитарные операторы

Посмотрим, какими свойствами обладают унитарные операторы и укажем, где это используется в физике.

Основные свойства (???)

$$\hat{A}|\lambda\rangle = \lambda|\lambda\rangle$$

$$\langle A\lambda|A\lambda\rangle = \langle \lambda|A^\dagger A\lambda\rangle = \langle\lambda|\lambda\rangle$$

$$\lambda^*\lambda\langle\lambda|\lambda\rangle = \langle\lambda|\lambda\rangle \quad \to \quad \lambda^*\lambda = 1$$

$$\lambda = \mathbf{e}^{i\phi}, \quad \phi \in \mathbb{R}(\mathrm{mod}[2\pi])$$

По сути мы доказали, что унитарный оператор представим в виде

$$\hat{A} = e^{\mathrm{i}\hat{\varphi}}, \quad \hat{\phi} = \hat{\phi}^\dagger,$$

наблюдаемые

если есть зависимость от параметра, то
можно пользоваться соотношениями *Фейнмана-Хеллмана*

$$\frac{\partial f_n}{\partial \lambda} = \left\langle n \left| \frac{\partial \hat{f}}{\partial \lambda} \right| n \right\rangle$$

Собственные функции и разложения

такое встречается и по сути это главное в анализе Гамильтониана!

вообще, по базису оператор раскладывать очень важно вроде бы, УМФ в том числе об этом, но я так и на освоил инструменты, как мы делаем все-таки это???

Другие методы с операторами

(остальное, что нужно или может быть нужно, тут.)

не разу не пригодилось, но в принципе звучит полезно:

можем раскладывать

$$f(\hat{O}) = f(0)\hat{\mathbb{I}} + \sum_{n=1}^{\infty} \frac{f^{(n)}(0)}{n!}\hat{O}^n$$

B.1.5 Matrices for Quantum Mechanics

мб про частичный след и тензорное произведение тут напишу (со ссылками на то, где это нужно).

(I'll shift it later to the theoretical sections!!!)

Матрицы Паули в квантовой механике

Основные свойства матриц Паули

Посмотрим на определение свойства матриц Паули.

Матрицы Паули по определению есть

$$\hat{\sigma}^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Их свойства:

$$\hat{\sigma}^\alpha \hat{\sigma}^\beta = \delta_{\alpha\beta}\hat{\mathbb{I}} + i\epsilon_{\alpha\beta\gamma}\hat{\sigma}^\gamma,$$

где $\alpha, \beta, \gamma \in \{x, y, z\}$.

доказывается легко просто вручную, но есть способ (в котором я забыл, что эти скобки значат? и который я пока не освоил, но он прямо лучший, мб.

хз.

короче, потом додумаю):

$$[\sigma_a, \sigma_b] = 2i\varepsilon_{abc}\sigma_c \qquad \{\sigma_a, \sigma_b\} = 2\delta_{ab}I,$$
$$[\sigma_a, \sigma_b] + \{\sigma_a, \sigma_b\} = (\sigma_a\sigma_b - \sigma_b\sigma_a) + (\sigma_a\sigma_b + \sigma_b\sigma_a)$$
$$2i\varepsilon_{abc}\sigma_c + 2\delta_{ab}I = 2\sigma_a\sigma_b$$

Также

$$e^{ia(\hat{n}\cdot\vec{\sigma})} = I\cos a + i(\hat{n}\cdot\vec{\sigma})\sin a$$

(тут я скипаю методы, вообще математику всю я потом думать буду)

$$\exp\left(ian_\alpha\hat{\sigma}^\alpha\right) = \cos a + in_\alpha\hat{\sigma}^\alpha \sin a$$

First let's see, that if $|\hat{n}| = 1$, we have

$$(\hat{n}\cdot\vec{\sigma})^{2p}=I.$$

If we sum three matrices $n_\alpha\sigma^\alpha$, we will have

$$M=\begin{pmatrix} n_3 & n_1-in_2 \\ n_1+in_2 & -n_3 \end{pmatrix}$$

and after multiplying $M\cdot M$, using $n_1^2+n_2^2+n_3^2=1$, we have $M^2=I$, so $(\hat{n}\cdot\vec{\sigma})^{2p}=I$. And this is the reason why

$$(\hat{n}\cdot\vec{\sigma})^{2q+1}=\hat{n}\cdot\vec{\sigma}$$

(нужно кстати научиться работать с экспонентой)

$$e^{ia(\hat{n}\cdot\vec{\sigma})}=\sum_{k=0}^{\infty}\frac{i^k[a(\hat{n}\cdot\vec{\sigma})]^k}{k!}=\sum_{p=0}^{\infty}\frac{(-1)^p(a\hat{n}\cdot\vec{\sigma})^{2p}}{(2p)!}+i\sum_{q=0}^{\infty}\frac{(-1)^q(a\hat{n}\cdot\vec{\sigma})^{2q+1}}{(2q+1)!}=$$
$$=I\sum_{p=0}^{\infty}\frac{(-1)^pa^{2p}}{(2p)!}+i(\hat{n}\cdot\vec{\sigma})\sum_{q=0}^{\infty}\frac{(-1)^qa^{2q+1}}{(2q+1)!}$$

interesting that

$$[\sigma_a,\sigma_b]+\{\sigma_a,\sigma_b\}=(\sigma_a\sigma_b-\sigma_b\sigma_a)+(\sigma_a\sigma_b+\sigma_b\sigma_a)$$

$$(\vec{a}\cdot\vec{\sigma})(\vec{b}\cdot\vec{\sigma})=(\vec{a}\cdot\vec{b})I+i(\vec{a}\times\vec{b})\cdot\vec{\sigma}$$

we need them because

$$\hat{H}=c\cdot\hat{\mathrm{I}}+b_x\sigma^x+b_y\sigma^y+b_z\sigma^z=c+(b,\hat{\sigma})$$

в общем, тема не раскрыта, написано много, а нужно от сюда хз, что, все нужно переусваивать, и мощь матриц паули я так и не понял.

Другие свойства матриц Паули

Тензорные произведения есть:

$$\hat{\sigma}_1^x\otimes\hat{\sigma}_2^x=\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix},\quad \hat{\sigma}_1^y\otimes\hat{\sigma}_2^y=\begin{pmatrix}0&0&0&-1\\0&0&1&0\\0&1&0&0\\-1&0&0&0\end{pmatrix},\quad \hat{\sigma}_1^y\otimes\hat{\sigma}_2^y=\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&1\end{pmatrix},$$

что легко выводится перемножением.

(а как явно будет в этом пространстве базис выглядеть?)

Появление матриц Паули

Покажем, каким образом появились матрицы Паули?

(пока завис вопрос, забыл немного, Киселев там выводил, потом сюда напишу. мб там несколько будет выводов?)

О применениях Матриц Паули

Во-первых, матрицы Паули нужны в записи оператора спина.
(формулы)
(здесь разберем подробно их пользу)

B.1.6 Tensor Operators

(I'll shift it later to the theoretical sections!!!)
(the idea is to give an intro to just mathematical side of this, but I'll write it first in the note on algebra, it is a very big topic)

определение и свойства

Дипольные сферические функции и циклические координаты $\mathcal{D}^1_{m',m}(\alpha,0,\beta)$

m'	1	0	-1
1	$\exp(-i(\alpha+\beta))$	0	0
0	0	1	0
-1	0	0	$\exp(i(\alpha+\beta))$

и еще таблица

m	$Y_{1,m}$	$rY_{1,m}$	r_m	$\vec{e}_m$
+1	$-\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi}$	$-\sqrt{\frac{3}{8\pi}}(x+iy)$	$-\frac{1}{\sqrt{2}}(x+iy)$	$-\frac{1}{\sqrt{2}}(\vec{e}_x+i\vec{e}_y)$
0	$\sqrt{\frac{3}{4\pi}}\cos\theta$	$\sqrt{\frac{3}{4\pi}}z$	z	$\vec{e}_z$
-1	$\sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\phi}$	$\sqrt{\frac{3}{8\pi}}(x-iy)$	$\frac{1}{\sqrt{2}}(x-iy)$	$\frac{1}{\sqrt{2}}(\vec{e}_x-i\vec{e}_y)$

r_m - циклические координаты радиуса-вектора;
p_m - циклические координаты импульса; J_m - циклические координаты углового момента; $J_{+1}=-\frac{1}{\sqrt{2}}J_+, \quad J_0=J_z, \quad J_{-1}=\frac{1}{\sqrt{2}}J_-$
Пусть $\Phi=T\Psi$. $R(\omega)\Phi=R(\omega)TR^{-1}(\omega)R(\omega)\Psi$
Если $\Psi=\Psi_{jm}$, то $R(\omega)\Psi_{jm}=\sum\limits_{n=-j}^{j}\mathcal{D}^j_{n,m}(\omega)\Psi_{jn}$

Набор из $(2k+1)$ операторов $T^k_q(k$ -целое или полуцелое неотрицательное число, $q=-k,-k+1,...,k-1,k)$ называется тензорным оператором ранга k, если при повороте тела (или системы координат) операторы T^k_q преобразуются так же как собственные функции операторов J^2 и $J_0\psi_{kq}$:

$$R(\omega)T^k_qR^{-1}(\omega)=\sum_{q'=-k}^{k}\mathcal{D}^k_{q',q}(\omega)T^k_{q'}$$

Примеры: ранг $k=1$ - операторы координаты, импульса, углового момента (их циклические координаты); ранг $k=L$ -сферические функции Y_{LM}, $M=-L,-L+1,...,L-1,L$

Покажите, что линейная комбинация тензорных операторов A^k и B^k ранга k есть тензорный оператор $\left(cA^k_q+dB^k_q, c \text{ и } d \text{ -числа}\right)$.

Теорема Вигнера-Эккарта

тут тупо по математике посмотрим все.
мб даже перекину в строгую квантовую механику.

формулировка

(потом)

$$\left\langle j'm' \left| T^k_q \right| jm \right\rangle = (-1)^{2k} \frac{\langle jmkq|j'm'\rangle}{\sqrt{2j'+1}} \left\langle j' \left\| T^k \right\| j \right\rangle$$

доказательство

(?? и в чем её идея???)

$$\begin{aligned}
\left\langle j'm' \left| T^k_q \right| jm \right\rangle &= \int \psi^*_{j'm'}(x) T^k_q(x) \psi_{jm}(x) dx = \\
&= \int \left(R(\omega)\psi_{j'm'}(x)\right)^* R(\omega) T^k_q(x) R^{-1}(\omega) R(\omega) \psi_{jm}(x) dx' = \\
&= \sum_{n',q',n} \int \overline{\mathcal{D}}^{j'}_{n',m'}(\omega) \psi^*_{j'm'}(x) \mathcal{D}^k_{q',q}(\omega) T^k_{q'}(x) \mathcal{D}^j_{n,m}(\omega) \psi_{jn}(x) dx = \\
&= \sum_{n',q',n} \overline{\mathcal{D}}^{j'}_{n',m'}(\omega) \mathcal{D}^k_{q',q}(\omega) \mathcal{D}^j_{n,m}(\omega) \left\langle j'n' \left| T^k_{q'} \right| jn \right\rangle .
\end{aligned}$$

Здесь мы (???? что сделали?? повращали зачем-то пространство???)

из какого-то домашнего задания:

$$\iiint \overline{\mathcal{D}}^{j}_{m,n}(\alpha,\beta,\gamma) \mathcal{D}^{j_1}_{m_1,n_1}(\alpha,\beta,\gamma) \mathcal{D}^{j_2}_{m_2,n_2}(\alpha,\beta,\gamma) \sin\beta d\beta d\gamma d\alpha =$$

$$= \frac{8\pi^2}{2j+1} \langle j_1 m_1 j_2 m_2 | jn \rangle \langle j_1 n_1 j_2 n_2 | jm \rangle$$

$$8\pi^2 \left\langle j'm' \left| T^k_q \right| jm \right\rangle = \langle jmkq|j'm'\rangle \sum_{n',q',n} \frac{8\pi^2}{2j'+1} \langle jnkq'|j'n'\rangle \left\langle j'n' \left| T^k_{q'} \right| jn \right\rangle$$

Матричный элемент тензорного оператора, вычисленный в обкладках функций с определёнными значениями j и m, можно представить в виде произведения коэффициента Клебша-Гордана и приведённого матричного элемента, который не зависит от магнитных квантовых чисел.

(??)

О применениях теоремы Вигнера-Эккарта

(?? хз)

Покажем простейшие случаи, где используется теорема Вигнера-Эккарта.

1.

Правила отбора по угловому моменту: $\triangle(j,k,j')$ и $m+q=m'$.

2.

Коэффициенты пересвязки $\left(\psi'_{jm}, \psi_{jm}\right) = \left(\psi'_{jm}, I\psi_{jm}\right) \sim \langle jm00|jm\rangle = 1$.

3.

Вероятность перехода системы из состояния $|j_1 m_1\rangle$ в состояние $|j_2 m_2\rangle$ под действием тензорного оператора T^k_q:

$$\frac{1}{2j_1+1}\sum_{m_1,m_2}\left|\left\langle j_2m_2\left|\sum_q T^k_q\right|j_1m_1\right\rangle\right|^2=\frac{1}{2j_1+1}\sum_{m_1,m_2,q_1,q_2}\langle j_1m_1kq_1|j_2m_2\rangle\times$$
$$\times\langle j_1m_1kq_2|j_2m_2\rangle\frac{1}{2j_2+1}\left\langle j_2\left\|T^k\right\|j_1\right\rangle^*\left\langle j_2\left\|T^k\right\|j_1\right\rangle=\frac{1}{2j_1+1}\left|\left\langle j_2\left\|T^k\right\|j_1\right\rangle\right|^2$$

Докажите эту формулу и вычислите (S и T - тензорные операторы)

$$\frac{1}{2j_1+1}\sum_{m_1,m_2}\left|\left\langle j_2m_2\left|\sum_{q_1}T^{k_1}_{q_1}+\sum_{q_2}S^{k_2}_{q_2}\right|j_1m_1\right\rangle\right|^2\text{ при }k_1\neq k_2$$

Тензорное произведение тензорных операторов

теория

(какие-то выгрузки, я хз вообще, мб когда-то посмотрю)

$$\left[U^{k_1}\times V^{k_2}\right]^k_q\equiv\sum_{q_1,q_2}\langle k_1q_1k_2q_2|kq\rangle\,U^{k_1}_{q_1}V^{k_2}_{q_2}$$

$$R(\omega)\left[U^{k_1}\times V^{k_2}\right]^k_qR^{-1}(\omega)=\sum_{q_1,q_2}\langle k_1q_1k_2q_2|kq\rangle\sum_{r_1,r_2}\mathcal{D}^{k_1}_{r_1,q_1}(\omega)\mathcal{D}^{k_2}_{r_2,q_2}(\omega)U^{k_1}_{r_1}V^{k_2}_{r_2}=$$

$$=\sum_{q_1,q_2}\frac{\langle k_1q_1k_2q_2|kq\rangle}{\sum\limits_{r_1,r_2}U^{k_1}_{r_1}V^{k_2}_{r_2}\sum\limits_{l,r}}\langle k_1r_1k_2r_2|lr\rangle\,\underline{\langle k_1q_1k_2q_2|lq\rangle}\mathcal{D}^l_{r,q}(\omega)=$$

$$=\sum_{r_1,r_2,r}\langle k_1r_1k_2r_2|kr\rangle\,U^{k_1}_{r_1}V^{k_2}_{r_2}\mathcal{D}^r_{r,q}(\omega)=\sum_r\mathcal{D}^r_{r,q}(\omega)\left[U^{k_1}\times V^{k_2}\right]^k_r$$

$$\left\langle aj'm'\left|\left[U^{k_1}\times V^{k_2}\right]^k_q\right|bjm\right\rangle=(-)^{2k}\frac{\langle jmkq|j'm'\rangle}{\sqrt{2j'+1}}\left\langle aj'\left\|\left[U^{k_1}\times V^{k_2}\right]^k\right\|bj\right\rangle$$

$$(-)^{2k}\left\langle aj'\left\|\left[U^{k_1}\times V^{k_2}\right]^k\right\|bj\right\rangle=\sqrt{2j'+1}\sum_{mq}\langle jmkq|j'm'\rangle\left\langle aj'm'\left|\left[U^{k_1}\times V^{k_2}\right]^k_q\right|bjm\right\rangle=$$

$$=\sqrt{2j'+1}\sum_{mq}\langle jmkq|j'm'\rangle\sum_{q_1q_2}\langle k_1q_1k_2q_2|kq\rangle\left\langle aj'm'\left|U^{k_1}_{q_1}V^{k_2}_{q_2}\right|bjm\right\rangle=$$

$$=\sqrt{2j'+1}\sum_{mq}\sum_{q_1q_2}\sum_{cJM}\langle jmkq|j'm'\rangle\langle k_1q_1k_2q_2|kq\rangle\left\langle aj'm'\left|U^{k_1}_{q_1}\right|cJM\right\rangle\left\langle cJM\left|V^{k_2}_{q_2}\right|bjm\right\rangle=$$

$$=\sqrt{2j'+1}\sum_{mq}\sum_{q_1q_2}\sum_{cJM}\langle jmkq|j'm'\rangle\langle k_1q_1k_2q_2|kq\rangle\times$$

$$\times(-)^{2k_1}\frac{\langle JMk_1q_1|j'm'\rangle}{\sqrt{2j'+1}}\left\langle aj'\left\|U^{k_1}\right\|cJ\right\rangle(-)^{2k_2}\frac{\langle jmk_2q_2|JM\rangle}{\sqrt{2J+1}}\left\langle cJ\left\|U^{k_1}\right\|bj\right\rangle=$$

$$=(-)^{2(k_1+k_2)}\sqrt{2j'+1}(-)^{j+k+j'}\sum_{cJ}\left\{\begin{array}{ccc}k_1&k_2&k\\j&j'&J\end{array}\right\}\left\langle aj'\left\|U^{k_1}\right\|cJ\right\rangle\left\langle cJ\left\|V^{k_2}\right\|bj\right\rangle$$
$$(-)^{2k}=(-)^{2(k_1+k_2)}$$

Коммутационные соотношения $J_0, J_\pm$ с тензорными операторами

$$R(\omega)T^k_q R^{-1}(\omega) = \sum_{r=-k}^{k} T^k_r \mathcal{D}^k_{r,q}(\omega)$$
$$\mathcal{D}^k_{r,q}(\omega) = (\psi_{j=k,m=r}, \exp(i\gamma J_0)\exp(i\beta J_y)\exp(i\alpha J_0)\,\psi_{j=k,m=q})$$

Покажите, рассмотрев бесконечно-малые повороты вокруг координатных осей, что (неприводимые) тензорные операторы должны удовлетворять коммутационным соотношениям

$$\left[J_0, T^k_q\right]_- = qT^k_q$$
$$\left[J_\pm, T^k_q\right]_- = \sqrt{(k\mp q)(k\pm q+1)}T^k_{q\pm1}$$

приведенные матричные элементы

(уже была эта часть теории выше, я все равно хз про это все)

$$Y_{l_1,m_1}(\theta,\phi)Y_{l_2,m_2}(\theta,\phi) = \sum_l \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}}\langle l_1m_1l_2m_2|lm\rangle\langle l_10l_20|l0\rangle Y_{l,m}(\theta,\phi)$$

$$\iint Y^*_{l,m}(\theta,\phi)Y_{l_2,m_2}(\theta,\phi)Y_{l_1,m_1}(\theta,\phi)\sin\theta d\theta d\phi = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi}}\frac{\langle l_1m_1l_2m_2|lm\rangle}{\sqrt{2l+1}}\langle l_10l_20|l0\rangle$$

$$\langle l\,\|Y_{l_2}\|\,l_1\rangle = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi}}\langle l_10l_20|l0\rangle; \quad \langle l\|1\|l_1\rangle = \delta(l-l_1)\sqrt{2l_1+1}$$

"Конструктор" для тензорных операторов

$$\left[U^{k_1}\times V^{k2}\right]^k_q = \sum_{q_1=-k_1}^{k_1}\sum_{q_2=-k_2}^{k_2}\langle k_1q_1k_2q_2|kq\rangle U^{k_1}_{q_1}V^{k_2}_{q_2}$$

$$\left\langle aj'\|\left[U^{k_1}\times V^{k_2}\int^k\|bj\right\rangle = (-)^{j+k+j'}\sqrt{2j'+1}\sum_{cJ}\left\{\begin{array}{ccc} k_1 & k_2 & k \\ j & j' & J\end{array}\right\}\left\langle aj'\left\|U^{k_1}\right\|cJ\right\rangle\left\langle cJ\left\|V^{k_2}\right\|bj\right\rangle$$

Скалярное произведение тензорных операторов

$$\left(U^k, V^k\right) \equiv \sum_{g=-k}^{k}(-)^qU^k_{-q}V^k_q$$

$$\left\langle bj'\left\|\left(U^k,V^k\right)\right\|aj\right\rangle = \frac{\delta(j'-j)}{\sqrt{2j+1}}\sum_{c,j_1}(-)^{j'-j_1}\left\langle bj'\left\|U^k\right\|cj_1\right\rangle\left\langle cj_1\left\|V^k\right\|aj\right\rangle$$

$$\left\langle bj'\|(\vec{A},\vec{J})\|aj\right\rangle = \frac{\delta(j'-j)}{\sqrt{2j+1}}\sum_{c,j_1}(-)^{j'-j_1}\left\langle bj'\|\vec{A}\|cj_1\right\rangle\left\langle cj_1\|\vec{J}\|aj\right\rangle =$$

$$= \frac{\delta(j'-j)}{\sqrt{2j+1}}\sum_{c,j_1}(-)^{j'-j_1}\left\langle bj'\|\vec{A}\|cj_1\right\rangle\delta(c-a)\delta(j_1-j)\sqrt{j(j+1)(2j+1)} =$$

$$= \delta\left(j'-j\right)\sqrt{j(j+1)}\left\langle bj'\|\vec{A}\|aj\right\rangle$$

$$= \delta\left(j'-j\right)\sqrt{j(j+1)}\left\langle bj'\|\vec{A}\|aj\right\rangle$$

в итоге:

$$\langle bj\|\vec{A}\|aj\rangle = \frac{1}{\sqrt{j(j+1)}}\langle bj\|(\vec{A},\vec{J})\|aj\rangle, \quad j>0$$

схемы связи тензорных операторов

Тензорное взаимодействие

$$V\left(r_{1,2}\right) = \left[\frac{\left(\vec{\sigma}_1,\vec{r}_{1,2}\right)\left(\vec{\sigma}_2,\vec{r}_{1,2}\right)}{r_{1,2}^2} - \frac{1}{3}\left(\vec{\sigma}_1,\vec{\sigma}_2\right)\right], \quad \vec{r}_{1,2} = \vec{r}_1 - \vec{r}_2$$

$$\left(\vec{\sigma}_1,\vec{r}_{1,2}\right)\left(\vec{\sigma}_2,\vec{r}_{1,2}\right) = 3\left[\sigma_1^1\times r_{1,2}^1\right]_0^0\left[\sigma_2^1\times r_{1,2}^1\right]_0^0 = 3\left[\left[\sigma_1^1\times r_{1,2}^1\right]^0\times\left[\sigma_2^1\times r_{1,2}^1\right]^0\right]_0^0 =$$

$$= 3\sum_{\lambda=0}^{2}(2\lambda+1)\left\{\begin{array}{ccc}1&1&0\\1&1&0\\\lambda&\lambda&0\end{array}\right\}\left[\left[\sigma_1^1\times\sigma_2^1\right]^\lambda\times\left[r_{1,2}^1\times r_{1,2}^1\right]^\lambda\right]_0^0 =$$

$$\lambda = 1: \quad \left[r_{1,2}^1\times r_{1,2}^1\right]^1 \sim \left[\vec{r}_{1,2}\times\vec{r}_{1,2}\right] = 0$$

$$\lambda = 0: \quad 3\left[\sigma_1^1\times\sigma_2^1\right]_0^0\left[r_{1,2}^1\times r_{1,2}^1\right]_0^0\frac{1}{3} = \frac{1}{3}\left(\vec{\sigma}_1,\vec{\sigma}_2\right)\left(\vec{r}_{1,2},\vec{r}_{1,2}\right) = \frac{1}{3}\left(\vec{\sigma}_1,\vec{\sigma}_2\right)r_{1,2}^2$$

$$= 3\left[\left[\sigma_1^1\times\sigma_2^1\right]^2\times\left[r_{1,2}^1\times r_{1,2}^1\right]^2\right]_0^0 5\left\{\begin{array}{ccc}1&1&0\\1&1&0\\2&2&0\end{array}\right\}$$

$$\left[\sigma_1^1\times\sigma_2^1\right]_m^2 = \Sigma_m^2, \quad \left[r_{1,2}^1\times r_{1,2}^1\right]_m^2 \sim r_{1,2}^2 Y_{2,m}\left(\theta_{1,2},\phi_{1,2}\right)$$

симметричные операторы

Переставим частицы в функции $\varphi(X)$

$$\left[DP^{-1}\varphi\right](X) = \int D\left(X,X'\right)\varphi\left(P^{-1}X'\right)dX' =$$
$$\text{замена переменных} \quad X'\to PX', \quad d\left(PX'\right) = dX'$$
$$= \int D\left(X,PX'\right)\varphi\left(X'\right)dX'$$
$$\left[PDP^{-1}\varphi\right](X) = \int D\left(PX,PX'\right)\varphi\left(X'\right)dX'$$

Ядро $D\left(PX,PX'\right)$ соответствует оператору PDP^{-1}, и наоборот.

Чтобы D не зависел от способа нумерации частиц, надо потребовать

$$D\left(PX,PX'\right) = D\left(X,X'\right) \text{ или } PDP^{-1} = D$$
$$PD = DP$$
$$PH - HP = 0 \text{ для любых перестановок } P.$$

действие на волновую функцию

T - транспозиция (перестановка между двумя неравными элементами).
$[H,T]_- = 0$.

$$T\varphi\left(x_1,x_2,...,x_N\right)=\lambda\varphi\left(x_1,x_2,...,x_N\right)$$
$$T^2\varphi\left(x_1,x_2,...,x_N\right)=\lambda^2\varphi\left(x_1,x_2,...,x_N\right)=\varphi\left(x_1,x_2,...,x_N\right),$$
$$\lambda^2=1,\quad \lambda=\pm1$$
$$\lambda=1:\quad T\varphi=\varphi,\quad P\varphi=\varphi$$
$$\lambda=-1:\quad T\varphi=-\varphi,\quad P\varphi=(-1)^P\varphi$$

$(-1)^P$ -четность перестановки (функция перестановки).

$$P\varphi=\varphi:\begin{cases}\text{симметричные функции; статистика "Бозе-Эйнштейна";}\\ \text{спин - ноль или целый; частицы - "бозоны".}\end{cases}$$
$$P\varphi=(-1)^P\varphi:\begin{cases}\text{антисимметричные функции; статистика "Ферми-Дирака";}\\ \text{спин - полуцелый; частицы - "фермионы".}\end{cases}$$

Симметричный одночастичный оператор

$$A-\ \text{одночастичный оператор};\quad A\rightleftharpoons A\left(x,x'\right)$$

A_j действует на j -ую частицу;

$$A_j\left(X,X'\right)=A\left(x_j,x'_j\right)\prod_{k\neq j}\delta\left(x'_k-x_k\right)$$

Если оператором P поменять местами j и i в $(x_1,...,x_N)$ и в $(x'_1,...,x'_N)$, то

$$A_j\left(PX,PX'\right)=A\left(x_i,x'_i\right)\prod_{k\neq i}\delta\left(x_k-x'_k\right)=A_i\left(X,X'\right)=A_{Pj}\left(X,X'\right)$$
$$PA_jP^{-1}=A_{Pj}$$
$$P\sum_{j=1}^{N}A_jP^{-1}=\sum_{j=1}^{N}A_{Pj}=\sum_{j=1}^{N}A_j$$
$$\mathfrak{A}\equiv\sum_{j=1}^{N}A_j$$
$$P\mathfrak{A}P^{-1}=\mathfrak{A}$$

Симметричный двухчастичный оператор

пока что я хз, что он делает и зачем он.
B действует на $\varphi(x,y)$

$$B\rightleftharpoons B\left(x,y;y',x'\right),\ \text{рассматриваем только:}\quad B\left(x,y;y',x'\right)=B\left(y,x;x',y'\right)$$

$$B_{j_1,j_2}\left(X,X'\right)=B\left(x_{j_1},x_{j_2};x'_{j_2},x'_{j_1}\right)\prod_{i\neq j_1,j_2}\delta\left(x'_i-x_i\right)$$

$$B_{j_2,j_1}\left(X,X'\right)=B_{j_1,j_2}\left(X,X'\right)$$

$$B_{j_1,j_2}\left(PX,PX'\right)=B_{Pj_1,Pj_2}\left(X,X'\right)\quad\rightleftharpoons\quad PB_{j_1,j_2}P^{-1}=B_{Pj_1,Pj_2}$$

$$\mathfrak{B} \equiv \sum_{1\le j_1<j_2\le N} B_{j_1,j_2} = \frac{1}{2}\sum_{1\le j_1,j_2\le N; j_1\ne j_2} B_{j_1,j_2}$$

$$P\mathfrak{B}P^{-1} = \frac{1}{2}\sum_{1\le j_1,j_2\le N; j_1\ne j_2} B_{Pj_1,Pj_2} = \frac{1}{2}\sum_{1\le j_1,j_2\le N; j_1\ne j_2} B_{j_1,j_2}$$

$$P\mathfrak{B}P^{-1} = \mathfrak{B}$$

$$\mathfrak{S}^{(s)} = \frac{1}{s!}\sum_{1\le j_1,j_2,\dots,j_s\le N; j_\alpha\ne j_\beta} S_{j_1,j_2,\dots,j_s}$$

B.1.7 Mathematical Analysis for Quantum Physics

также неплохо в отдельном месте разобраться с тем, как решаем мы просто математические задачи.

и тут основные методы решения я запишу.

обзор применений в квантовой физике

гипергеометрическая функция

обзор ее применений

вкратце теория

гипергеометрическая функция и атом водорода

приведем эту связь.

полиномы Эрмита

обзор ее применений

в линейном осцилляторе решение как раз через них и идет.

$$H_n(z) = (-1)^n e^{z^2}\frac{d^n}{dz^n}\left(e^{-z^2}\right)$$

вкратце теория

B.1.8 Integrals

пока просто буду собирать, потом пойму, что в каком месте нужно

$$e^{-iA^2} = \frac{e^{i\pi/4}}{\sqrt{\pi}}\int\limits_{-\infty}^{\infty} dz e^{iz^2-2izA}$$

обзор применений ТФКП в квантовой физике

метод перевала

суть метода перевала

Пусть зафиксирован некоторый контур; и нам требуется найти асимптотики функции $y(x \to \pm\infty)$. Эту задачу отлично решает метод перевала, который применяется к интегралам вида:

$$y = \int\limits_C A(z)e^{\Phi(z)}dz$$

С вещественным методом перевала мы уже сталкивались; если функция $\Phi(z)$ чисто вещественна на контуре интегрирования, то достаточно найти максимумы этой функции $\Phi'(z_0) = 0$, разложиться квадратично вблизи этих максимумов (а медленную огибающую $A(z)$ можно просто взять в максимуме $A(z_0)$). Метод перевала в комплексной плоскости базируется на этой же простой идее, и он использует то хорошее свойство комплексных интегралов от аналитических функций, а именно - возможность модифицировать контур интегрирования.

Таким образом, для асимптотической оценки интеграла всегда модифицировать контур так, чтобы уходить только по линиям постоянной фазы $\mathrm{Im}\Phi\ (z) = \mathrm{const}$.

Обратим внимание, что линии постоянной фазы тождественно совпадают с линиями жаискорейшего спуска, то есть с направлением $\nabla Re\Phi$.

реализация метода перевала

??? пойму его, потом потренируюсь.

(по птф пока что алгоритм выписал)

Шаг первый Сперва требуется найти положение так называемых седловых точек $^{13}\Phi'(z_0) = 0$. В напем случае есть функция $\Phi(t) = xt - \frac{t^3}{3} \to \Phi' = x - t^2 = 0$. При $x > 0$, имеется пара седловых точек на вещественной оси $t_{1,2} = \pm\sqrt{x}$; при $x < 0$ имеется пара седловых точек на мнимой оси $t_{3,4} = \pm i\sqrt{|x|}$. Определим сразу значения функции в этих седловых точках:

$$\Phi(t) = \begin{cases} \pm\frac{2}{3}x^{3/2}, & t = t_{1,2} = \pm\sqrt{x} \\ \mp\frac{2}{3}i|x|^{3/2} & t = t_{3,4} = \pm i\sqrt{|x|} \end{cases}$$

Шаг второй Затем требуется найти направление линий наискорейпего спуска из точки z_0. Вблизи каждой точки функция в общем виде раскладывается квадратично $\Phi(z) \approx \Phi(z_0) + \frac{1}{2}\Phi''(z_0)\cdot(z - z_0)^2 + \ldots$. Рассмотрим поведение функции $\mathrm{Re}\,\Phi(z)$ в окрестности z_0; если положить $\Phi'' = |\Phi''|\, e^{i\arg\Phi''}$ и $z - z_0 = \rho e^{i\theta}$, тогда $\mathrm{Re}\,(\Phi(z) - \Phi(z_0)) = \frac{1}{2}|\Phi''|\,\rho^2 e^{i(\arg\Phi'' + 2\theta)}$

Имеются следующие взаимно-перпендикулярные направления: $\arg\Phi'' + 2\theta = 2\pi n \to \theta = -\frac{1}{2}\arg\Phi''$, $\theta = -\frac{1}{2}\arg\Phi'' + \pi$ (направления наискорейшего возрастания) $\arg\Phi'' + 2\theta = \pi + 2\pi n \to \theta = -\frac{1}{2}\arg\Phi'' \pm \frac{\pi}{2}$, (направления наискорейпего спуска) В нашем случае получается следующее:

$$\Phi''(t) = -2t = \begin{cases} -2\sqrt{x} \to \theta = 0, \pi, & t_1 = \sqrt{x}, \quad x > 0 \\ 2\sqrt{x} \to \theta = \pm\frac{\pi}{2} & t_2 = -\sqrt{x}, \quad x > 0 \\ -2i\sqrt{|x|} \to \theta = -\frac{\pi}{4}, \frac{3\pi}{4}, & t_3 = i\sqrt{|x|}, \quad x < 0 \\ 2i\sqrt{|x|} \to \theta = -\frac{3\pi}{4}, \frac{\pi}{4}, & t_4 = -i\sqrt{|x|}, \quad x < 0 \end{cases}$$

Шаг третий Таким образом, нам бы хотелось пустить контур через точку z_0 под углом, соответствующим линии постоянной фазы - линии наискорейшего спуска.

Если мы поступим так, то вклад в интеграл от окрестности z_0 оденится следующим образом [14]:

$$y = \int\limits_C dz A(z) e^{-\Phi(z)} \approx \int\limits_{-\infty}^{\infty} e^{i\theta} d\rho A(z) e^{\Phi(z_0) - \frac{1}{2}|\Phi''|\rho^2} = \sqrt{\frac{2\pi}{|\Phi''|}} A\left(z_0\right) e^{\Phi(z_0)+i\theta}$$

Обратим внимание, что ведущая зависимость от параметра, как правило, даётся просто посредством $e^{\Phi(z_0)}$. Конечно, тут предполагается выполнение стандартных критериев метода перевала (а именно, что максимум достаточно узкий, и функция $A(z)$ достаточно медленна, так что такое разложение оправдано).

выбрать контур, соответствующий функции Эйри

Шаг четвёртый Теперь нам можно наконец выбрать контур, соответствуюпий функции Эйри.

Функция Эйри определяется как вещественное решение, которое при $x > 0$ экспоненциально затухает.

Поэтому при $x > 0$ контур должен проходить только через седловую точку t_2, и никак не через t_1. Такой контур единственный - это C_1 (контур, идущий из нижнего сектора в верхний).

Для удобства его можно пустить чисто по мнимой оси; выбирая константу так, чтобы определение совпало с стандартным (она равна $\frac{1}{2\pi i}$), мы можем написать:

$$\mathrm{Ai}(x) = \frac{1}{2\pi i} \int\limits_{C_1} e^{xt - t^3/3} dt = \frac{1}{\pi} \int\limits_0^{\infty} \cos\left(xt - \frac{t^3}{3}\right) dt$$

Шаг пятый Теперь проведём непосредственно перевальную оценку интеграла по выбранному контуру для различных знаков x. При $x > 0$, контур кнасаживается на единственную седловую точку $t = t_2 = -\sqrt{x}$ и проходит через неё по направлению $\theta = \frac{\pi}{2}$; получается вклад:

$$\mathrm{Ai}(x \to \infty) \approx \frac{1}{2\sqrt{\pi} x^{1/4}} e^{-\frac{2}{3}x^{3/2}}$$

При $x < 0$ контур насаживается на обе седловые точки.

Однако стоит обратить внимания, что фазы в них различны $\mathrm{Im}\,\Phi\left(t_3\right) \neq \mathrm{Im}\,\Phi\left(t_4\right)$;

в связи с этим, вообще говоря, не существует единого контура, который проходит по линиям постоянной фазы через обе седловые точки.

В действительности же контур идёт кснизуж, проходит через седло $t = -2i\sqrt{|x|}$ под углом $\theta = \frac{\pi}{4}$; затем уходит на $t \to +\infty$ (подобно контуру $-C_3$!).

Там он перескакивает на другую линию постоянной фазы, откуда от возвращается по ней до второго седла $t = 2i\sqrt{|x|}$, проходит его под направлением $\theta = \frac{3\pi}{4}$ и уходит кнаверх (как контур $-C_2$; смотри рисунок 4.2). Перевальная оценка тем самьгм даёт:

$$\mathrm{Ai}(x \to -\infty) \approx \frac{1}{2\pi i} \sqrt{\frac{2\pi}{2\sqrt{|x|}}} \left[e^{\frac{2}{3}i|x|^{3/2} i\frac{\pi}{4}} + e^{-\frac{2}{3}i|x|^{3/2} + i\frac{3\pi}{4}} \right] = \frac{1}{\sqrt{\pi}|x|^{1/4}} \sin\left(\frac{2}{3}|x|^{3/2} + \frac{\pi}{4}\right)$$

Template integrals, which are very useful for some problems

Полезные математические заготовки для стационарной теории возмущений в невырожденном случае

Обсудим интегралы и другие нужные преобразования.

Всегда сперва проверяем по компу формулой типа:

```
Integrate[(Sin[2 Pi x/ a ])^2 x^2, {x, 0, a }]
```

(??? какая-то фигня у вольфрама с двойными интегралами, так что считаю их по отдельности.)

Далее, если считаем руками, то используем полезные заготовки неопределенного интеграла:

$$\int \sin^2(Cx)\,dx = \frac{x}{2} - \frac{\sin(2Cx)}{4C},$$
$$\int \sin^2(Cx)\,xdx = x^2/4 - \frac{\cos[2Cx]}{8C^2} - \frac{x\sin[2Cx]}{4C},$$
$$\int \sin^2(Cx)\,x^2dx = x^3/6 - \frac{x\cos[2Cx]}{4C^2} - \frac{(-1+2C^2x^2)\sin[2Cx]}{8C^3},$$
$$\int \sin^2(\pi Cx)\,x^3dx = x^4/8 - (3(-1+2C^2x^2)\cos[2Cx])/(16C^4) - (x(-3+2C^2x^2)\sin[2Cx])/(8C^3),$$

И определенного интеграла:

$$\int_0^a \sin^2\left(\pi\frac{x}{a}\right)dx = \frac{a}{2},$$
$$\int_0^a \sin^2\left(\pi\frac{x}{a}\right)xdx = \frac{a^2}{4},$$
$$\int_0^a \sin^2\left(\pi\frac{x}{a}\right)x^2dx = \frac{1}{12}a^3(2-\frac{3}{\pi^2}),$$
$$\int_0^a \sin^2\left(\pi\frac{x}{a}\right)x^3dx = (a^4(-3+\pi^2))/(8\pi^2),$$
$$\int_0^a \sin\left(2\pi\frac{x}{a}\right)\sin\left(\pi\frac{x}{a}\right)x = -\frac{8a^2}{9\pi^2},$$

(добавлю потом другие)

B.1.9 Iterative Methods

просто можно делать какие-то итерационные решения, тут про них я изучу все

$$1 = \frac{maU_0}{\sqrt{2m|E|}}2\ln\frac{1}{\sqrt{2m|E|}a} \qquad \leftrightarrow \qquad \frac{a\sqrt{2m|E|}}{ma^2U_0} = -2\ln\sqrt{2m|E|}a \tag{B.1}$$

Засунем мелкость в параметр $\beta = ma^2U_0 \ll 1$.
(я пока что хз, зачем, но еще вводим) $\alpha := a\sqrt{2m|E|}/\beta$.
в итоге начинаем эту хрень писать:

$$\alpha = -2\ln(\alpha\beta) \tag{B.2}$$
$$\alpha_0 = 1 \ \rightarrow \tag{B.3}$$
$$\alpha_1 = -2\ln(\beta) \ \rightarrow \tag{B.4}$$
$$\alpha_2 = -2\ln(-2\beta\ln(\beta)) \tag{B.5}$$
$$\tag{B.6}$$

то есть глава посвящена ответу на вопрос: какого хрена так происходит????

C Programming for Quantum Mechanics

Обсудим приложения квантовой механики в программировании.

(раздел на страниц 30, соберу все методы в вольфраме проги, которые уже написаны у Шмиеда "вольфрам в квантмехе". также про квантовое машинное обучение и всё такое, это тут)

C.1 Modeling of Typical Objects and Phenomena

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References

[1] Poboiko I., Antonenko D., Stepanov N.: *Seminars on quantum mechanics at the landau institute*. 2020.

[2] Griffiths, David J. and Schroeter, Darrell F.: *Introduction to Quantum Mechanics*. Cambridge University Press, 3rd edition, 2018.

[3] Киселёв, В.В.: *Квантовая механика. Курс лекций ч. 1*. 2005.

[4] Киселёв, В. В.: *Квантовая механика. Курс лекций ч. 2*. 2005.

[5] Zhou, K.: *Lecture Notes on Undergraduate Physics*. 2022. https://knzhou.github.io/notes/phy.pdf.

[6] Кингсеп, А. С, Белонучкин В. Е., Заикин Д. А., Ципенюк, Ю. М.: *Основы физики т.2 квантовая физика и термодинамика*. 2007.

[7] Galitski, V.M., Karnakov, B., Galitski, V., and Kogan, V.I.: *Exploring Quantum Mechanics: A Collection of 700+ Solved Problems for Students, Lecturers, and Researchers*. OUP Oxford, 2013, ISBN 9780199232727. https://books.google.be/books?id=NwrdQHswYwkC.

[8] Белоусов, Ю. М.: *Задачи по теоретической физике*.

[9] Тахтаджян, Л. А.: *Квантовая механика для математиков*. Ижевск: НИЦ «Регулярная и хаоти ческая динамика», Ижевский институт компью терных исследований, 2011.

[10] Зинн-Жюстен Ж.: *Континуальный интеграл в квантовой механике*. 2010.

[11] Nielsen, M. A., Chuang, I. L.: *Quantum Computation and Quantum Information: 10th Anniversary Edition*. Cambridge University Press, USA, 10th edition, 2011, ISBN 1107002176.

[12] Базь, А. И., Зельдович, Я. Б., Переломов, А. М. : *Рассеяние, реакции и распады в нерелятивистской квантовой механике*. 1971.

[13] Landau, L.D. and Lifshitz, E.M.: *Quantum Mechanics: Non-Relativistic Theory*. Course of theoretical physics. Butterworth-Heinemann, 1991, ISBN 9780750635394. https://books.google.si/books?id=J9ui6KwC4mMC.

[14] Behtash, Alireza, Dunne, Gerald V, Schäfer, Thomas, Sulejmanpasic, Tin, and Unsal, Mithat: *Toward picard-lefschetz theory of path integrals, complex saddles and resurgence*. arXiv preprint arXiv:1510.03435, 2015.

[15] Kleinert H.: *Path integrals in quantum mechanics, statistics, polymer physics, and financial markets*. World scientific, 2009.

[16] Дирак, П. А. М.: *Лекции по квантовой механике*. М.–Ижевск: НИЦ «Регулярная и хаотическая динамика, page 148, 1998.

[17] Tomonaga, S.: *The Story of Spin*. A Pacific Basin Institute book. University of Chicago Press, 1997, ISBN 9780226807942. https://books.google.bg/books?id=he9sANipCj8C.

[18] Соловьев, В. Г.: *Теория ядра. Модели ядер*. Энергоиздат, 1981.

[19] Бор О., Моттельсон Б.: *Структура атомного ядра т. 1*. 1971.

[20] Schmied, R.: *Using Mathematica for Quantum Mechanics A Student's Manual*.

[21] Мессиа, А.: *Квантовая механика*. Энергоиздат, 1958.

[22] G., Baumann: *Mathematica for theoretical physics: classical mechanics and nonlinear dynamics*, volume 1. Springer Science & Business Media, 2006.

[23] Ландау Л. Д., Лифшиц Е. М., Берестецкий В. Б.: *Квантовая электродинамика*. 1989.

[24] Sakurai, J.J., Napolitano, J.: *Modern Quantum Mechanics*. Addison-Wesley, 2011, ISBN 9780805382914. https://books.google.bg/books?id=N4I-AQAACAAJ.

[25] Littlejohn, R.: *Physics 221ab: Quantum mechanics*.

[26] Igoshin F.F., Samarskiy Yu. A., Tsipenyuk Yu. M.: *Laboratory practice in general physics. Quantum physics: A textbook for universities*. M.: Fizmatkniga, ISBN 978-5-89155-206-7.

[27] Левитов Л. С., Шитов А. В.: *Функция Гнина. Задачи и Решения*.

[28] Sivukhin D. V.: *General Physics course: Atomic Physics. vol. V.[in Russian]*. M.: Nauka.

[29] М., Каку: *Физика невозможного*. Альпина Паблишер, 2011.

[30] Каку, М.: *Параллельные миры: Об устройстве мироздания, высших измерениях и будущем Космоса*. Альпина Паблишер, 2017.

[31] Иванов, М. Г.: *Как понимать квантовую механику*. М.–Ижевск: НИЦ «Регулярная и хаотическая динамика, page 550, 2012.

[32] Фейнман Р. Ф.: *Квантовая электродинамика*. Либроком, 2008.

[33] Мухин, К. Н.: *Занимательная ядерная физика*. Рипол Классик, 1972.

[34] фон Нейман, И.: *Математические основы квантовой механики*. Наука.

[35] Халфин, Л.А.: *Квантовый эффект Зенона*. Успехи физических наук, 160(10):185–188, 1990.

[36] Purcell, E. M: *Proceedings of the american physical society: Spontaneous emission probabilities at ratio frequencies*. Jun 1946. https://link.aps.org/doi/10.1103/PhysRev.69.674.2.

[37] Aharonov, Yakir, Albert, David Z., and Vaidman, Lev: *How the result of a measurement of a component of the spin of a spin-1/2 particle can turn out to be 100*. Phys. Rev. Lett., 60:1351–1354, Apr 1988. https://link.aps.org/doi/10.1103/PhysRevLett.60.1351.

[38] Hubač, Ivan and Wilson, Stephen: *Brillouin-Wigner Methods for Many-Body Systems*, volume 21. December 2009, ISBN 978-90-481-3372-7.

[39] Bravyi S., DiVincenzo D. P., Loss D.: *Schrieffer–Wolff transformation for quantum many-body systems*. Annals of Physics, 326(10):2793–2826, oct 2011. https://doi.org/10.1016%2Fj.aop.2011.06.004.

[40] Feldbrugge J, Pen U., Turok N.: *Oscillatory path integrals for radio astronomy*, 2019. https://arxiv.org/abs/1909.04632.

[41] Spaldin, N. A.: *Magnetic Materials: Fundamentals and Applications*. Cambridge University Press, 2nd edition, 2010.

[42] Боголюбов Н.Н., Боголюбов Н.Н. (мл.).: *Введение в квантовую статистическую механику Изд. 3*. ISBN 978-5-9710-4456-7.

[43] Бор О., Моттельсон Б.: *Структура атомного ядра т. 2*. 1977.

Bibliography from Takhtajan

[AM78] R. Abraham and J.E. Marsden, Foundations of mechanics, Benjamin/Cummings Publishing Co. Inc., Reading, MA, 1978.
[AG93] N.I. Akhiezer and I.M. Glazman, Theory of linear operators in Hilbert space, Dover Publications Inc., New York, 1993.
[AHK76] S.A. Albeverio and R.J. Hegh-Krohn, Mathematical theory of Feynman path integrals, Lecture Notes in Mathematics, vol. 523, Springer-Verlag, Berlin, 1976.
[AE05] S.T. Ali and M. Engli, Quantization methods: a guide for physicists and analysts, Rev. Math. Phys. 17 (2005), no. 4, 391-490.
[AG83] L. Alvarez-Gaum, Supersymmetry and the Atiyah-Singer index theorem, Comm. Math. Phys. 90 (1983), no. 2, 161-173.
[ASW90] O. Alvarez, I.M. Singer, and P. Windey, Quantum mechanics and the geometry of the Weyl character formula, Nuclear Phys. B 337 (1990), no. 2, 467-486.
[Alv95] O. Alvarez, Lectures on quantum mechanics and the index theorem, Geometry and quantum field theory (Park City, UT, 1991), IAS/Park City Math. Ser., vol. 1, Amer. Math. Soc., Providence, RI, 1995, pp. 271-322.
[Apo76] T.M. Apostol, Introduction to analytic number theory, Undergraduate Texts in Mathematics, Springer-Verlag, New York, 1976.
[Arn89] V.I. Arnol'd, Mathematical methods of classical mechanics, Graduate Texts in Mathematics, vol. 60, Springer-Verlag, New York, 1989.
[AG90] V.I. Arnol'd and A.B. Givental', Symplectic geometry, Dynamical systems IV, Encyclopaedia of Mathematical Sciences, vol. 4, Springer-Verlag, Berlin, 1990, pp. 1-136.
[AKN97] V.I. Arnol'd, V.V. Kozlov, and A.I. Neishtadt, Mathematical aspects of classical and celestial mechanics, Encyclopaedia of Mathematical Sciences, vol. 3, Springer-Verlag, Berlin, 1997.
[Ati85] M.F. Atiyah, Circular symmetry and stationary-phase approximation, Astrisque (1985), no. 131, 43-59, Colloquium in honor of Laurent Schwartz, Vol. 1 (Palaiseau, 1983).
[BI66a] M. Bander and C. Itzykson, Group theory and the hydrogen atom. Part I, Rev. Mod. Phys. 38 (1966), 330-345.
[BI66b] , Group theory and the hydrogen atom. Part II, Rev. Mod. Phys. 38 (1966), 346-358.
[Bar61] V. Bargmann, On a Hilbert space of analytic functions, Comm. Pure Appl. Math. 3 (1961), 215-228.
[BR86] A.O. Barut and R. Rczka, Theory of group representations and applications, second ed., World Scientific Publishing Co., Singapore, 1986.
[BW97] S. Bates and A. Weinstein, Lectures on the geometry of quantization, Berkeley Mathematics Lecture Notes, vol. 8, Amer. Math. Soc., Providence, RI, 1997.

[BFF+78a] F. Bayen, M. Flato, C. Fronsdal, A. Lichnerowicz, and D. Sternheimer, Deformation theory and quantization. I. Deformations of symplectic structures, Ann. Physics 111 (1978), no. 1, 61-110.
[BFF+78 b] ..., Deformation theory and quantization. II. Physical applications, Ann. Physics 111 (1978), no. 1, 111-151.
[Bel87] J.S. Bell, Speakable and unspeakable in quantum mechanics, Collected papers on quantum philosophy, Cambridge University Press, Cambridge, 1987.
[Ber61] F.A. Berezin, Canonical operator transformation in representation of secondary quantization, Soviet Physics Dokl. 6 (1961), 212-215 (in Russian).
[Ber66] __ The method of second quantization, Pure and Applied Physics, vol. 24, Academic Press, New York, 1966.
[Ber71a] __ Non-Wiener path integrals, Teoret. Mat. Fiz. 6 (1971), no. 2, 194212 (in Russian), English translation in Theoret. and Math. Phys. 6 (1971), 141-155.
[Ber71b] , Wick and anti-Wick symbols of operators, Mat. Sb. (N.S.) 86(128) (1971), 578-610 (in Russian), English translation in Math. USSR Sb. 15 (1971), 577-606.
[Ber74] , Quantization, Izv. Akad. Nauk SSSR Ser. Mat. 38 (1974), 1116-1175 (in Russian), English translation in Math. USSR-Izv. 78 (1974), 1109-1165.
[Ber87] _ , Introduction to superanalysis, Mathematical Physics and Applied Mathematics, vol. 9, D. Reidel Publishing Co., Dordrecht, 1987.
[BS91] F.A. Berezin and M.A. Shubin, The Schrdinger equation, Mathematics and its Applications (Soviet Series), vol. 66, Kluwer Academic Publishers Group, Dordrecht, 1991.
[BGV04] N. Berline, E. Getzler, and M. Vergne, Heat kernels and Dirac operators, Corrected reprint of the 1992 original, Grundlehren Text Editions, SpringerVerlag, Berlin, 2004.
[BS87] M.Sh. Birman and M.Z. Solomjak, Spectral theory of selfadjoint operators in Hilbert space, Mathematics and its Applications (Soviet Series), D. Reidel Publishing Co., Dordrecht, 1987.
[Bis84a] J.-M. Bismut, The Atiyah-Singer theorems: a probabilistic approach. I. The index theorem, J. Funct. Anal. 57 (1984), no. 1, 56-99.
[Bis84b] __ The Atiyah-Singer theorems: a probabilistic approach. II. The Lefschetz fixed point formulas, J. Funct. Anal. 57 (1984), no. 3, 329-348.
[Bis85] _ Index theorem and equivariant cohomology on the loop space, Comm. Math. Phys. 98 (1985), no. 2, 213-237.
[BT95] M. Blau and G. Thompson, Localization and diagonalization: a review of functional integral techniques for low-dimensional gauge theories and topological field theories, J. Math. Phys. 36 (1995), no. 5, 2192-2236.
[Bry95] R.L. Bryant, An introduction to Lie groups and symplectic geometry, Geometry and quantum field theory (Park City, UT, 1991), IAS/Park City Math. Ser., vol. 1, Amer. Math. Soc., Providence, RI, 1995, pp. 5-181.
[BFK91] D. Burghelea, L. Friedlander, and T. Kappeler, On the determinant of elliptic differential and finite difference operators in vector bundles over S^1, Comm. Math. Phys. 138 (1991), no. 1, 1-18.
[BFK95] , On the determinant of elliptic boundary value problems on a line segment, Proc. Amer. Math. Soc. 123 (1995), no. 10, 3027-3038.
[BF60] V.S. Buslaev and L.D. Faddeev, Formulas for traces for a singular SturmLiouville differential operator, Dokl. Akad. Nauk. SSSR 132 (1960), 13-16 (in Russian), English translation in Soviet Math. Dokl. 1 (1960), 451-454.
[Cam63] R.H. Cameron, The Ilstow and Feynman integrals, J. Analyse Math. 10 (1962/1963), 287-361.
[Cra83] M. Crampin, Tangent bundle geometry for Lagrangian dynamics, J. Phys. A 16 (1983), no. 16, 3755-3772.

[CFKS08] H.L. Cycon, R.G. Froese, W. Kirsch, and B. Simon, Schrdinger operators with application to quantum mechanics and global geometry, Corrected and extended 2nd printing, Texts and Monographs in Physics, Springer-Verlag, Berlin, 2008.
[Dav76] A.S. Davydov, Quantum mechanics, International Series in Natural Philosophy, vol. 1, Pergamon Press, Oxford, 1976.
[DEF +99] P. Deligne, P. Etingof, D.S. Freed, L.C. Jeffrey, D. Kazhdan, J.W. Morgan, D.R. Morrison, and E. Witten (eds.), Quantum fields and strings: a course for mathematicians. Vol. 1, 2, Amer. Math. Soc., Providence, RI, 1999, Material from the Special Year on Quantum Field Theory held at the Institute for Advanced Study, Princeton, NJ, 1996-1997.
[DF99a] P. Deligne and D.S. Freed, Classical field theory, Quantum fields and strings: a course for mathematicians, Vol. 1, 2 (Princeton, NJ, 1996/1997), Amer. Math. Soc., Providence, RI, 1999, pp. 137-225.
[DF99b] _ Supersolutions, Quantum fields and strings: a course for mathematicians, Vol. 1, 2 (Princeton, NJ, 1996/1997), Amer. Math. Soc., Providence, RI, 1999, pp. 227-355.
[DM99] P. Deligne and J.W. Morgan, Notes on supersymmetry (following J. Bernstein), Quantum fields and strings: a course for mathematicians, Vol. 1, 2 (Princeton, NJ, 1996/1997), Amer. Math. Soc., Providence, RI, 1999, pp. 4197.
[Dik58] L.A. Diki1, Trace formulas for Sturm-Liouville differential operators, Uspekhi Mat. Nauk (N.S.) 13 (1958), no. 3(81), 111-143 (in Russian), English translation in Amer. Math. Soc. Transl. (2) 18 (1961), 81-115.
[Dir47] P.A.M. Dirac, The principles of quantum mechanics, Clarendon Press, Oxford, 1947.
[DR01] W. Dittrich and M. Reuter, Classical and quantum dynamics. From classical paths to path integrals, third ed., Advanced Texts in Physics, Springer-Verlag, Berlin, 2001.
[Dri83] V.G. Drinfel'd, Constant quasiclassical solutions of the Yang-Baxter quantum equation, Dokl. Akad. Nauk SSSR 273 (1983), no. 3, 531-535 (in Russian), English translation in Soviet Math. Dokl. 28 (1983), 667-671.
[Dri86] ——, Quantum groups, Zap. Nauchn. Sem. Leningrad. Otdel. Mat. Inst. Steklov. (LOMI) 155 (1986), 18-49 (in Russian), English translation in J. Soviet Math. 41 (1988), no. 2, 898-915.
[Dri87] , Quantum groups, Proceedings of the International Congress of Mathematicians, Vol. 1, 2 (Berkeley, Calif., 1986) (Providence, RI), Amer. Math. Soc., 1987, pp. 798-820.
[DFN84] B.A. Dubrovin, A.T. Fomenko, and S.P. Novikov, Modern geometry methods and applications. Part I, Graduate Texts in Mathematics, vol. 93, Springer-Verlag, New York, 1984.
[DFN85] _, Modern geometry - methods and applications. Part II, Graduate Texts in Mathematics, vol. 104, Springer-Verlag, New York, 1985.
[Dyn98] A. Dynin, A rigorous path integral construction in any dimension, Lett. Math. Phys. 44 (1998), no. 4, 317-329.
[Enr01] B. Enriquez, Quantization of Lie bialgebras and shuffle algebras of Lie algebras, Selecta Math. (N.S.) 7 (2001), no. 3, 321-407.
[Erd56] A. Erdlyi, Asymptotic expansions, Dover Publications Inc., New York, 1956.
[EK96] P. Etingof and D. Kazhdan, Quantization of Lie bialgebras. I, Selecta Math. (N.S.) 2 (1996), no. 1, 1-41.
[Fad57] L.D. Faddeev, An expression for the trace of the difference between two singular differential operators of the Sturm-Liouville type, Dokl. Akad. Nauk SSSR (N.S.) 115 (1957), 878-881 (in Russian).
[Fad59] _ The inverse problem in the quantum theory of scattering, Uspekhi Mat. Nauk 14 (1959), no. 4 (88), 57-119 (in Russian), English translation in J. Math. Phys. 4 (1963), 72–104.
[Fad64], Properties of the S-matrix of the one-dimensional Schrdinger equation, Trudy Mat. Inst. Steklov. 73 (1964), 314-336 (in Russian), English translation in Amer. Math. Soc. Transl. (2), Vol. 65: Nine papers on partial differential equations and functional analysis

(1967), 139-166.
[Fad74] The inverse problem in the quantum theory of scattering. II, Current problems in mathematics, Vol. 3, Akad. Nauk SSSR Vsesojuz. Inst. Naun. i Tehn. Informacii, Moscow, 1974, pp. 93-180 (in Russian), English translation in J. Soviet Math. 5 (1976), no. 3, 334-396.
[Fad76] Course 1. Introduction to functional methods, Mthodes en thorie des champs/Methods in field theory (cole d't Phys. Thor., Session XXVIII, Les Houches, 1975), North-Holland, Amsterdam, 1976, pp. 1-40.
[Fad98] , A mathematician's view of the development of physics, Les relations entre les mathmatiques et la physique thorique, Inst. Hautes tudes Sci., Bures, 1998, pp. 73-79.
[Fad99] , Elementary introduction to quantum field theory, Quantum fields and strings: a course for mathematicians, Vol. 1, 2 (Princeton, NJ, 1996/1997), Amer. Math. Soc., Providence, RI, 1999, pp. 513-550.
[FY80] L.D. Faddeev and O.A. Yakubovskii, Lectures on quantum mechanics for mathematics students, Leningrad University Publishers, Leningrad, 1980 (in Russian).
[FS91] L.D. Faddeev and A.A. Slavnov, Gauge fields. Introduction to quantum theory, Frontiers in Physics, vol. 83, Addison-Wesley Publishing Company, Redwood City, CA, 1991.
[FT07] L.D. Faddeev and L.A. Takhtajan, Hamiltonian methods in the theory of solitons, Reprint of 1987 English edition, Classics in Mathematics, SpringerVerlag, New York, 2007.
[Fey48] R.P. Feynman, Space-time approach to non-relativistic quantum mechanics, Rev. Modern Physics 20 (1948), 367-387.
[Fey51] , An operator calculus having applications in quantum electrodynamics, Physical Rev. (2) 84 (1951), 108-128.
[FH65] R.P. Feynman and A.R. Hibbs, Quantum mechanics and path integrals, McGraw Hill, New York, 1965.
[Fla82] M. Flato, Deformation view of physical theories, Czechoslovak J. Phys. B32 (1982), 472-475.
[Foc32] V.A. Fock, Konfigurationsraum und zweite Quantelung, Z. Phys. 75 (1932), no. 9-10, 622-647.
[Foc78] ., Fundamentals of quantum mechanics, Mir Publishers, Moscow, 1978.
[Fre99] D.S. Freed, Five lectures on supersymmetry, Amer. Math. Soc., Providence, RI, 1999.
[Fuj80] D. Fujiwara, Remarks on convergence of the Feynman path integrals, Duke Math. J. 47 (1980), no. 3, 559-600.
[FH91] W. Fulton and J. Harris, Representation theory, Graduate Texts in Mathematics, vol. 129, Springer-Verlag, New York, 1991.
[GL53] I.M. Gel'fand and B.M. Levitan, On a simple identity for the characteristic values of a differential operator of the second order, Dokl. Akad. Nauk SSSR (N.S.) 88 (1953), 593-596 (in Russian).
[GY56] I.M. Gel'fand and A.M. Yaglom, Integration in function spaces and its application to quantum physics, Uspekhi Mat. Nauk (N.S.) 11 (1956), no. 1(67), 77-114, English translation in J. Math. Phys. 1 (1960), 48-69.
[Ger50] Ya.L. Geronimus, Teoriya ortogonal'nyh mnogolenov, Gosudarstv. Izdat. Tehn.-Teor. Lit., Moscow-Leningrad, 1950 (in Russian).
[Gi195] P.B. Gilkey, Invariance theory, the heat equation, and the Atiyah-Singer index theorem, second ed., CRC Press, Boca Raton, FL, 1995.
[God69] C. Godbillon, Gometrie differntielle et mcanique analytique, Hermann, Paris, 1969.
[GK69] I.C. Gohberg and M.G. Krein, Introduction to the theory of linear nonselfadjoint operators, Translations of Mathematical Monographs, Vol. 18, Amer. Math. Soc., Providence, RI, 1969.
[Gol80] H. Goldstein, Classical mechanics, Addison Wesley, 1980.
[GW98] R. Goodman and N.R. Wallach, Representations and invariants of the classical groups,

Encyclopedia of Mathematics and its Applications, vol. 68, Cambridge University Press, Cambridge, 1998.
[GS77] V. Guillemin and S. Sternberg, Geometric asymptotics, Mathematical Surveys, No. 14, Amer. Math. Soc., Providence, RI, 1977.
[GS03] S.J. Gustafson and I.M. Sigal, Mathematical concepts of quantum mechanics, Universitext, Springer-Verlag, Berlin, 2003.
[HS96] P.D. Hislop and I.M. Sigal, Introduction to spectral theory: With applications to Schrdinger operators, Applied Mathematical Sciences, vol. 113, SpringerVerlag, New York, 1996.
[IM74] K. It and H.P. McKean, Jr., Diffusion processes and their sample paths, Second printing, corrected, Die Grundlehren der mathematischen Wissenschaften, Band 125, Springer-Verlag, Berlin, 1974.
[IZ80] C. Itzykson and J.B. Zuber, Quantum field theory, International Series in Pure and Applied Physics, McGraw-Hill International Book Co., New York, 1980.
[Jim85] M. Jimbo, A q-difference analogue of $U(\mathfrak{g})$ and the Yang-Baxter equation, Lett. Math. Phys. 10 (1985), no. 1, 63-69.
[JW28] P. Jordan and E. Wigner, ber das Paulische Aquivalenzverbot, Z. Phys. 47 (1928), 631-658.
[Kac59] M. Kac, Probability and related topics in physical sciences, Lectures in Applied Mathematics. Proceedings of the Summer Seminar, Boulder, CO, 1957, vol. 1, Interscience Publishers, London-New York, 1959.
[Kac80] _ , Integration in function spaces and some of its applications, Lezioni Fermiane, Accademia Nazionale dei Lincei, Pisa, 1980.
[Kaz99] D. Kazhdan, Introduction to QFT, Quantum fields and strings: a course for mathematicians, Vol. 1, 2 (Princeton, NJ, 1996/1997), Amer. Math. Soc., Providence, RI, 1999, pp. 377-418.
[Kho07] D. Khoshnevisan, Probability, Graduate Studies in Mathematics, vol. 80, Amer. Math. Soc., Providence, RI, 2007.
[Kir76] A.A. Kirillov, Elements of the theory of representations, Grundlehren der Mathematischen Wissenschaften, Band 220, Springer-Verlag, Berlin, 1976.
[Kir90] _ Geometric quantization, Dynamical systems IV, Encyclopaedia of Mathematical Sciences, vol. 4, Springer-Verlag, Berlin, 1990, pp. 137-172.
[Kir04] , Lectures on the orbit method, Graduate Studies in Mathematics, vol. 64, Amer. Math. Soc., Providence, RI, 2004.
[KSV02] A.Yu. Kitaev, A.H. Shen, and M.N. Vyalyi, Classical and quantum computation, Graduate Studies in Mathematics, vol. 47, Amer. Math. Soc., Providence, RI, 2002.
[Kon03] M. Kontsevich, Deformation quantization of Poisson manifolds, Lett. Math. Phys. 66 (2003), no. 3, 157-216.
[Kos77] B. Kostant, Graded manifolds, graded Lie theory, and prequantization, Differential geometrical methods in mathematical physics (Proc. Sympos., Univ. Bonn, Bonn, 1975), Lecture Notes in Math., vol. 570, Springer-Verlag, Berlin, 1977.
[Kre62] M.G. Kren, On perturbation determinants and a trace formula for unitary and self-adjoint operators, Dokl. Akad. Nauk SSSR 144 (1962), 268-271 (in Russian), English translation in Soviet Math. Dokl. 3 (1962), 707-710.
[LL58] L.D. Landau and E.M. Lifshitz, Quantum mechanics: non-relativistic theory. Course of Theoretical Physics, Vol. 3, Pergamon Press Ltd., London-Paris, 1958.
[LL76] L.D. Landau and E.M. Lifshitz, Mechanics. Course of theoretical physics. Vol. 1, Pergamon Press, Oxford, 1976.
[Lan87] S. Lang, Elliptic functions, second ed., Springer-Verlag, New York, 1987.
[Ler81] J. Leray, Lagrangian analysis and quantum mechanics, A mathematical structure re-

lated to asymptotic expansions and the Maslov index, MIT Press, Cambridge, MA, 1981.
[LS91] B.M. Levitan and I.S. Sargsjan, Sturm-Liouville and Dirac operators, Mathematics and its Applications (Soviet Series), vol. 59, Kluwer Academic Publishers Group, Dordrecht, 1991.
[LV80] G. Lion and M. Vergne, The Weil representation, Maslov index and theta series, Progress in Mathematics, vol. 6, Birkhuser, Boston, MA, 1980.
[Lo77] M. Love, Probability theory. I, fourth ed., Graduate Texts in Mathematics, vol. 45, Springer-Verlag, New York, 1977.
[Lo78] _ , Probability theory. II, fourth ed., Graduate Texts in Mathematics, vol. 46, Springer-Verlag, New York, 1978.
[Mac04] G.W. Mackey, Mathematical foundations of quantum mechanics, Reprint of the 1963 original, Dover Publications Inc., Mineola, NY, 2004.
[Man97] Y.I. Manin, Gauge field theory and complex geometry, second ed., Grundlehren der Mathematischen Wissenschaften, vol. 289, Springer-Verlag, Berlin, 1997.
[Mar86] V.A. Marchenko, Sturm-Liouville operators and applications, Operator Theory: Advances and Applications, vol. 22, Birkhuser Verlag, Basel, 1986.
[Mar59a] J.L. Martin, The Feynman principle for a Fermi system, Proc. Roy. Soc. Ser. A 251 (1959), no. 1267, 543-549.
[Mar59b] Generalized classical dynamics, and the 'classical analogue' of a Fermi oscillator, Proc. Roy. Soc. Ser. A 251 (1959), no. 1267, 536-542.
[MF81] V.P. Maslov and M.V. Fedoriuk, Semiclassical approximation in quantum mechanics, Mathematical Physics and Applied Mathematics, vol. 7, D. Reidel Publishing Co., Dordrecht, 1981.
[Mes99] A. Messiah, Quantum mechanics, Dover Publications Inc., Mineola, NY, 1999.
[MP49] S. Minakshisundaram and Å. Pleijel, Some properties of the eigenfunctions of the Laplace-operator on Riemannian manifolds, Canadian J. Math. 1 (1949), 242-256.
[Mon52] E.W. Montroll, Markoff chains, Wiener integrals, and quantum theory, Comm. Pure Appl. Math. 5 (1952), 415-453.
[Nel59] E. Nelson, Analytic vectors, Ann. of Math. (2) 70 (1959), 572-615.
[Nel64] , Feynman integrals and the Schrdinger equation, J. Math. Phys. 5 (1964), 332-343.
[New02] R.G. Newton, Scattering theory of waves and particles, Reprint of the 1982 second edition, with list of errata prepared by the author, Dover Publications Inc., Mineola, NY, 2002.
[Olv97] F.W.J. Olver, Asymptotics and special functions, Reprint of the 1974 original, AKP Classics, A K Peters Ltd., Wellesley, MA, 1997.
[PW35] L. Pauling and E.B. Wilson, Introduction to quantum mechanics. With applications to chemistry, McGraw-Hill Book Company, New York and London, 1935.
[Rab95] J.M. Rabin, Introduction to quantum field theory for mathematicians, Geometry and quantum field theory (Park City, UT, 1991), IAS/Park City Math. Ser., vol. 1, Amer. Math. Soc., Providence, RI, 1995, pp. 183-269.
[RS71] D.B. Ray and I.M. Singer, R-torsion and the Laplacian on Riemannian manifolds, Advances in Math. 7 (1971), 145-210.
[RS80] M. Reed and B. Simon, Methods of modern mathematical physics. I, Academic Press, New York, 1980.
[RS75] _ , Methods of modern mathematical physics. II. Fourier analysis, selfadjointness, Academic Press, New York, 1975.
[RS79] , Methods of modern mathematical physics. III. Scattering theory, Academic Press, New York, 1979.
[RS78] , Methods of modern mathematical physics. IV. Analysis of operators, Academic Press, New York, 1978.
[RTF89] N.Yu. Reshetikhin, L.A. Takhtadzhyan, and L.D. Faddeev, Quantization of Lie groups and Lie algebras, Algebra i Analiz 1 (1989), no. 1, 178-206 (in Russian), English translation in

Leningrad Math. J. 1 (1990), 193-225.
[Ros04] J. Rosenberg, A selective history of the Stone-von Neumann theorem, Operator algebras, quantization, and noncommutative geometry, Contemp. Math., vol. 365, Amer. Math. Soc., Providence, RI, 2004, pp. 331-353.
[RSS94] G.V. Rozenblyum, M.Z. Solomyak, and M.A. Shubin, Spectral theory of differential operators, Partial differential equations. VII, Encyclopaedia of Mathematical Sciences, vol. 64, Springer-Verlag, Berlin, 1994.
[Rud87] W. Rudin, Real and complex analysis, third ed., McGraw-Hill Book Co., New York, 1987.
[Sak94] J.J. Sakurai, Modern quantum mechanics, Addison-Wesley Publishing Company, 1994.
[See67] R.T. Seeley, Complex powers of an elliptic operator, Singular Integrals (Proc. Sympos. Pure Math., Chicago, IL, 1966), Amer. Math. Soc., Providence, RI, 1967, pp. 288-307.
[STS85] M.A. Semenov-Tian-Shansky, Dressing transformations and Poisson group actions, Publ. Res. Inst. Math. Sci. 21 (1985), no. 6, 1237-1260.
[SW76] D.J. Simms and N.M.J. Woodhouse, Lectures in geometric quantization, Lecture Notes in Physics, 53, Springer-Verlag, Berlin, 1976.
[Ste83] S. Sternberg, Lectures on differential geometry, second ed., Chelsea Publishing Co., New York, 1983.
[Str05] F. Strocchi, An introduction to the mathematical structure of quantum mechanics. A short course for mathematicians, Advanced Series in Mathematical Physics, vol. 27, World Sci. Publishing, London-Singapore, 2005.
[Sza00] R.J. Szabo, Equivariant cohomology and localization of path integrals, Lecture Notes in Physics. New Series: Monographs, vol. 63, Springer-Verlag, Berlin, 2000.
[Sze75] G. Szeg, Orthogonal polynomials, Amer. Math. Soc., Providence, RI, 1975.
[Tak90] L. A. Takhtajan, Lectures on quantum groups, Introduction to quantum group and integrable massive models of quantum field theory (Nankai, 1989), Nankai Lectures Math. Phys., World Sci. Publishing, River Edge, NJ, 1990, pp. 69197.
[Tob56] W. Tobocman, Transition amplitudes as sums over histories, Nuovo Cimento (10) 3 (1956), 1213-1229.
[Var04] V.S. Varadarajan, Supersymmetry for mathematicians: an introduction, Courant Lecture Notes in Mathematics, vol. 11, New York University Courant Institute of Mathematical Sciences, New York, 2004.
[Vil68] N.Ja. Vilenkin, Special functions and the theory of group representations, Translations of Mathematical Monographs, Vol. 22, Amer. Math. Soc., Providence, RI, 1968.
[vN31] J. von Neumann, Die Eindeutigkeit der Schrdingershen Operatoren, Mathematische Annalen 104 (1931), 570-578.
[vN96] _, Mathematical foundations of quantum mechanics, Princeton Landmarks in Mathematics, Princeton University Press, Princeton, NJ, 1996.
[Vor05] A.A. Voronov, Notes on universal algebra, Graphs and patterns in mathematics and theoretical physics (Stony Brook, NY, 2001), Proc. Sympos. Pure Math., vol. 73, Amer. Math. Soc., Providence, RI, 2005, pp. 81-103.
[Wey50] H. Weyl, Theory of groups and quantum mechanics, Dover Publications, New York, 1950.
[Wig59] E.P. Wigner, Group theory: And its application to the quantum mechanics of atomic spectra, Pure and Applied Physics, Vol. 5, Academic Press, New York, 1959.
[Wit82a] E. Witten, Constraints on supersymmetry breaking, Nuclear Phys. B 202 (1982), no. 2, 253-316.
[Wit82b] , Supersymmetry and Morse theory, J. Differential Geom. 17 (1982), no. 4, 661-692 (1983).
[Wit99a] , Homework, Quantum fields and strings: a course for mathematicians, Vol. 1,

2 (Princeton, NJ, 1996/1997), Amer. Math. Soc., Providence, RI, 1999, pp. 609-717.
[Wit99b] , Index of Dirac operators, Quantum fields and strings: a course for mathematicians, Vol. 1, 2 (Princeton, NJ, 1996/1997), Amer. Math. Soc., Providence, RI, 1999, pp. 475-511.
[Woo92] N.M.J. Woodhouse, Geometric quantization, second ed., Oxford Mathematical Monographs, The Clarendon Press Oxford University Press, New York, 1992.
[Yaf92] D.R. Yafaev, Mathematical scattering theory. General theory, Translations of Mathematical Monographs, vol. 105, Amer. Math. Soc., Providence, RI, 1992.
[YI73] K. Yano and S. Ishihara, Tangent and cotangent bundles: differential geometry, Pure and Applied Mathematics, No. 16, Marcel Dekker Inc., New York, 1973.

Refs from Quantum mechanics of the $1/x^2$ potential by Essin, Griffiths (2005)

[4] K. S. Gupta and S. G. Rajeev, "Renormalization in quantum mechanics," Phys. Rev. D 48, 5940-5945 (1993).
[5] G. Arfken and H.-J. Weber, Mathematical Methods for Physicists (Academic, Orlando (2000), 5th ed., Chap. 11. The other solution, $\sqrt{x}I_{ig}(\kappa x)$, diverges for large x.
[6] I. S. Gradshteyn and I. M. Ryzhik, Tables of Integrals, Series, and Products (Academic, San Diego, (1980), Eqs. (6.576.4) and (8.332.3). Incidentally, states with different κ are not orthogonal.
[7] One might ask what the usual approximation schemes have to say about this potential. Not much. For the general power law $V(x) = ax^\nu$ on $0 < x < \infty$, the WKB approximation yields $E_n \approx a[(n - 1/4)\hbar\sqrt{2\pi/ma}\Gamma(1/\nu + 3/2)/\Gamma(1/\nu + 1)]^{2\nu/(\nu+2)}$ [see D. J. Griffiths, Introduction to Quantum Mechanics (Prentice Hall, Englewood Cliffs, NJ, 2004), 2nd ed., Problem 8.11], and the exponent is infinite when $\nu = -2$. The variational principle only confirms what we already knew-that the ground state is lower than every negative energy.
[8] Reference 6, p. 962, Eqs. (3) and (4).
[9] Some authors use a plus sign in Eq. (24), which adds $\pi/2$ to the phase shift. We prefer the minus sign, because it reduces to $\delta = 0$ when the potential is zero.
[10] For a list of accessible references see C. V. Siclen, "The one-dimensional hydrogen atom," Am. J. Phys. 56, 9-10 (1988).
[11] Indeed, because allowed energies must exceed $V_{\min}, E_1 > -a/\epsilon^2$.
[12] For these parameters $\kappa_1\epsilon = 1.024645, \kappa_2\epsilon = 0.350972, \kappa_3\epsilon = 0.122830$, and $\kappa_4\epsilon = 0.043089$.
[13] For the ground state this inequality would appear to require $g \ll 3$ (see Fig. 5), but in practice the approximation is good up to $g = 3$. For the excited states κ is smaller, and the approximation is valid for even higher g.
[14] Reference 5, Eqs. (11.112) and (11.118), and Ref. 6, Eqs. (8.331) and (8.332).
[15] This holds for $g < 3$, as we can easily confirm by comparing the graph of Eq. (30) with Fig. 5. For larger values of g the approximation itself is invalid for the ground state. Incidentally, Eq. (29) has solutions for negative n, but these are spurious, because they violate the assumption $\kappa\epsilon < 1$.
[16] The limiting case $g = 0$ is obviously problematic-indeed, $K_0(z)$ has no zeros for positive z. For $|z| \ll 1, \Gamma(1 + z) \approx 1 - Cz$, where $C = 0.577215$ is Euler's constant, so for small g arg $\Gamma(1 + ig) \approx -Cg$, and Eq. (30) is replaced by $\kappa_n = (2/\gamma\epsilon)\exp(-n\pi/g)$, where $\gamma \equiv \exp(C) = 1.781072$. See Ref. 6, Eq. (8.321.1), and p. xxviii.
[17] We used the identity $H_{ig}^{(2)}(x) = \left[H_{-ig}^{(1)}(x)\right]^* = e^{-\pi g}\left[H_{ig}^{(1)}(x)\right]^*$ (valid for real x and real g). See Ref. 6, p. 969.
[18] We used Ref. 6, Eq. (8.405.1), to express $H_\nu^{(1)}$ in terms of J_ν and N_ν, Eq. (8.440) to approximate J_v, Eq. (8.443) to approximate N_v, and Eq. (8.332.3) to eliminate $\Gamma(1 - ig)$.
[19] Reference 6, Eqs. (8.331) and (8.332.1).

[20] Reference 6, Eqs. (8.441.1) and (8.444.1), and p. xxviii.

(then, there were just comments)
[27] H. Weyl, "Über gewöhnliche Differentialgleichungen mit Singularitäten und die zugehörigen Entwicklungen willkürlicher Funktionen," Math. Ann. 68, 220-269 (1910); J. von Neumann, "Allgemeine Eigenwerttheorie Hermitescher Funktionaloperatoren," ibid. 102, 49-131 (1929); M. H. Stone, "On one-parameter unitary groups in Hilbert space," Ann. Math. 33, 643-648 (1932).
[28] N. I. Akhiezer and I. M. Glazman, Theory of Linear Operators in Hilbert Space (Dover, New York, 1993); M. Reed and B. Simon, Methods of Modern Mathematical Physics (Academic, London, 1975); G. Hellwig, Differential Operators of Mathematical Physics (Addison-Wesley, Reading, MA, 1964).
[29] G. Bonneau, J. Faraut, and G. Valent, "Self-adjoint extensions of operators and the teaching of quantum mechanics," Am. J. Phys. 69, 322-331 (2001).
[30] V. S. Araujo, F. A. B. Coutinho, and J. F. Perez, "Operator domains and self-adjoint operators," Am. J. Phys. 72, 203-213 (2004).
[31] There exist pathological functions that are square-integrable and yet do
not go to zero at infinity, but there is no penalty for excluding them here. See, for example, D. V. Widder, Advanced Calculus (Dover, New York, 1998), 2nd ed., p. 325.

(then, there were just comments)
[43] C. Zhu and J. R. Klauder, "Classical symptoms of quantum illnesses," Am. J. Phys. 61, 605-611 (1993); N. A. Wheeler, "Relativistic classical fields," unpublished notes, Reed College, 1973, pp. 246-251.
[44] J.-M. Lévy-Leblond, "Electron capture by polar molecules," Phys. Rev. 153, 1-4 (1967).
[45] M. H. Mittleman and V. P. Myerscough, "Minimum moment required to bind a charged particle to an extended dipole," Phys. Lett. 23, 545-546 (1966); W. B. Brown and R. E. Roberts, "On the critical binding of an electron by an electric dipole," J. Chem. Phys. 46, 2006-2007 (1966).
[46] C. Desfrançois, H. Abdoul-Carime, N. Khelifa, and J. P. Schermann, "From $1/r$ to $1/r^2$ potentials: Electron exchange between Rydberg atoms and polar molecules," Phys. Rev. Lett. 73, 2436-2439 (1994); Coon and Holstein (Ref. 1); many articles by H. E. Camblong and collaborators, especially "Quantum anomaly in molecular physics," Phys. Rev. Lett. 87, 220402-1-4 (2001).

From Chaos and the semiclassical limit of quantum mechanics (is the moon there when somebody looks?) by Berry

1. Berry, M. V.,1983, Semiclassical Mechanics of regular and irregular motion in Les Houches Lecture Series eds. G.Iooss, R.H.G.Helleman & R.Stora (North Holland, Amsterdam), Vol. 36, pp. 171-271.

2. Berry, M. V.,1987, Quantum chaology (The Bakerian Lecture) Proc. Roy. Soc. Lond. A413, 183-198.

3. Gutzwiller, M. C.,1990, Chaos in classical and quantum mechanics (Springer, New York).

4. Schuster, H. G., 1988, Deterministic Chaos. An introduction (VCH Verlagsgesellschaft, Weinheim).

5. Wilson, E. O.,1998, Consilience: The Unity of Knowledge (Knopf, New York).

6. Berry, M. V.,1994, Asymptotics, singularities and the reduction of theories in Proc. 9th Int. Cong. Logic, Method., and Phil. of Sci. eds. Prawitz, D., Skyrms, B. & Westerståhl, D., pp. 597-607.

7. Fuchs, C. & Peres, A.,2000, Quantum theory needs no 'Interpretation' Physics Today, 70-71.

8. Berry, M. V.,1991, Some quantum-to-classical asymptotics in Chaos and Quantum Physics, Les Houches Lecture Series eds. Giannoni, M.-J., Voros, A. & Zinn-Justin, J. (North-Holland, Amsterdam), Vol. 52, pp. 251-304.

9. Russell, B. & Whitehead, A. N., 2nd ed),1927, Principia Mathematica (University Press, Cambridge).

10. Wisdom, J., S.J., P. & Mignard, F., 1984, The chaotic rotation of Hyperion Icarus 58, 137-152.

11. Black, G. J., Nicholson, P. D. & Thomas, P. C.,1995, Hyperion: Rotational dynamics Icarus 117, 149-161.

12. Casati, G., Chirikov, B. V., Ford, J. & Izraelev, F. M.,1979, in Stochastic Behaviour in Classical and Quantum Hamiltonian Systems, eds. G.Casati & J.Ford, Vol. 93, pp. 334-352.

13. Berry, M. V., Balazs, N. L., Tabor, M. & Voros, A.,1979, Quantum maps Ann. Phys. N.Y. 122, 26-63.

14. Korsch, H. J. & Berry, M. V.,1981, Evolution of Wigner's phasespace density under a non-integrable quantum map Physica 3D, 627-636.

15. Omnes, R.,1992, Consistent interpretations of quantum-mechanics Revs Mod. Phys. 64, 339-382.

16. Omnes, R.,1997, General theory of the decoherence effect in quantum mechanics Phys. Rev. A 56, 3383-3394.

17. Zurek, W. H. & Paz, J. P.,1994, Decoherence, chaos and the 2nd law Phys. Rev. Lett. 72, 2508-2511.

18. Zurek, W. H. & Paz, J. P.,1995, Quantum chaos - a decoherent definition PHYSICA D 83, 300-308.

19. Zurek, W. H., 1998, Decoherence, chaos, quantum-classical correspondence, and the algorithmic arrow of time Physica Scripta 76, 186-198.

20. Fishman, S., Grempel, D. R. & Prange, R. E.,1982, Chaos, quantum recurrences, and Anderson localization Phys. Rev. Lett. 49, 509-512.

21. Braun, D., Haake, F. & Strunz, W.,2000, Universality of decoherence Preprint, University of Essen.

22. Harris, R. A. & Stodolsky, L., 1978, Quantum beats in optical activity and weak interactions Phys. Lett. B. 78B, 313-317.

23. Harris, R. A. & Stodolsky, L., 1982, Two state systems in media and "Turing's Paradox" Phys. Lett. 116B, 464-469.

24. Harris, R. A. & Silbey, R.,1983, On the stabilization of optical isomers through tunneling friction J.Chem. Phys. 78, 7330-7333.

25. Pfeifer, P.,1980, in Chemistry (ETH, Zürich).

26. Pascazio, S., Namiki, M., Badurek, G. & Rauch, H.,1993, Quantum Zeno effect with neutron spin Phys. Lett. A 179, 155-160.

27. Nakazato, H., Namiki, M., Pascazio, S. & Yamanaka, Y.,1996, Quantum dephasing by chaos Physics Letters A 222, 130-136.

28. Berry, M. V.,1995, Some two-state quantum asymptotics in Fundamental Problems of quantum theory eds. Greenberger, D. M. & Zeilinger, A. (Ann. N.Y. Acad. Sci., Vol. 255, pp. 303-317.

29. Facchi, P., Pascazio, S. & Scardicchio, A.,1999, Measurementinduced quantum diffusion Phys. Rev. Lett. 83, 61-64.

30. Berry, M. V.,1981, Singularities in Waves and rays in Les Houches Lecture Series Session 35 eds. Balian, R., Kléman, M. & Poirier, J.-P. (North-Holland: Amsterdam, pp. 453-543.

31. Nye, J. F.,1999, Natural focusing and fine structure of light: Caustics and wave dislocations (Institute of Physics Publishing, Bristol).

32. Arnold, V. I., 1986, Catastrophe Theory (Springer, Berlin).

33. Poston, T. & Stewart, I.,1978, Catastrophe theory and its applications (Pitman (reprinted by Dover), London).

34. Berry, M. V.,1976, Waves and Thom's theorem Advances in Physics 25, 1-26.

35. Berry, M. V. & Upstill, C., 1980, Catastrophe optics: morphologies of caustics and their diffraction patterns Progress in Optics 18, 257-346.

36. Nye, J. F. & Berry, M. V.,1974, Dislocations in wave trains Proc. Roy. Soc. Lond. A336, 165-90.

37. Nye, J. F., 1981, The motion and structure of dislocations in wavefronts Proc. Roy. Soc. Lond. A378, 219-239.

38. Berry, M. V. & Dennis, M. R.,2000, Phase singularities in isotropic random waves Proc. Roy. Soc. Lond. A.

39. Soskin, M. S., 1997, in SPIE (Optical Society of America, Washington), Vol. 3487.

40. Vasnetsov, M. & Staliunas, K.,1999, (Nova Science Publications, Commack, New York).

41. Nye, J. F.,1983, Polarization effects in the diffraction of electromagnetic waves: the role of disclinations. Proc. Roy. Soc. Lond. A387, 105-132.

42. Nye, J. F., 1983, Lines of circular polarization in electromagnetic wave fields Proc. Roy. Soc. Lond. A389, 279-290.

43. Nye, J. F. & Hajnal, J. V.,1987, The wave structure of monochromatic electromagnetic radiation Proc. Roy. Soc. Lond. A409, 21-36.

44. Berry, M. V. & Tabor, M.,1977, Level clustering in the regular spectrum Proc. Roy. Soc. Lond. A356, 375-94.

45. Bohigas, O. & Giannoni, M. J.,1984, in Mathematical and Computational Methods in Nuclear Physics, eds. J.S.Dehesa, J.M.G.Gomez & A.Polls (Springer-Verlag, Vol. 209, pp. 1-99.

46. Bohigas, O., Giannoni, M. J. & Schmit, C.,1984, Characterization of chaotic quantum spectra and universality of level fluctuation laws Phys. Rev. Lett. 52, 1-4.

47. Haake, F.,1991, Quantum signatures of chaos (Springer-Verlag, Heidelberg).

48. Berry, M. V.,1981, Quantizing a classically ergodic system: Sinai's billiard and the KKR method Ann. Phys. 131, 163-216.

49. Porter, C. E., 1965, Statistical Theories of Spectra Fluctuations (Adademic Press, New York).

50. Mehta, M. L., 1967, Random Matrices and the Statistical Theory of Energy Levels (Academic Press, New York and London).

51. Scharf, R., Dietz, B., Kus, M., Haake, F. & Berry, M. V.,1988, Kramers' degeneracy and quartic level repulsion Europhys. Lett. 5, 383-389.

52. Seligman, T. H., Verbaarschot, J. J. M. & Zirnbauer, M. R.,1985, Spectral fluctuation properties of Hamiltonian systems: the transition region between order and chaos J. Phys. A 18, 27512770.

53. Berry, M. V. & Robnik, M.,1986, Statistics of energy levels without time-reversal symmetry: Aharonov-Bohm chaotic billiards J. Phys. A 19, 649-668.

54. Berry, M. V. & Mondragon, R. J.,1987, Neutrino billiards: timereversal symmetry-breaking without magnetic fields Proc. Roy. Soc. Lond. A412, 53-74.

55. Berry, M. V.,1985, Semiclassical theory of spectral rigidity Proc. Roy. Soc. Lond. A400, 229-251.

56. Keating, J. P., 1992, Periodic-orbit resummation and the quantization of chaos Proc. Roy. Soc. Lond A436, 99-108.

57. Bogomolny, E. B. & Keating, J. P., 1996, Gutzwiller's trace formula and spectral statistics: beyond the diagonal approximation Phys. Rev. Lett. 77, 1472-1475.

58. Argaman, N., Dittes, F. M., Doron, E., Keating, J. P., Kitaev, A., Sieber, M. & Smilansky, U.,1992, Correlations in the actions of periodic orbits derived from quantum chaos Phys. Rev. Lett. 71, 4326-4329.

59. Keating, J. P., 1994, Long-time divergence of semiclassical formfactors J. Phys. A. 27, 6605-6615.

60. Berry, M. V. & Keating, J. P., 1999, The Riemann zeros and eigenvalue asymptotics SIAM Review 41, 236-266.

61. Berry, M. V., 1988, Semiclassical formula for the number variance of the Riemann zeros Nonlinearity 1, 399-407.

62. Berry, M. V. & Keating, J. P., 1992, A new approximation for zeta(1/2+it) and quantum spectral determinants Proc. Roy. Soc. Lond. A437, 151-173.

63. Keating, J. P.,1993, The Riemann zeta-function and quantum chaology in Quantum Chaos eds. Casati, G., Guarneri, I. & Smilansky, U. (North-Holland, Amsterdam), pp. 145-185.

64. Keating, J. P. & Sieber, M.,1994, Calculation of spectral determinants Proc. Roy. Soc. Lond. A447, 413-437.

65. Bogomolny, E. B. & Keating, J. P.,1995, Random matrix theory and the Riemann zeros I: three- and four-point correlations Nonlinearity 8, 1115-1131.

66. Bogomolny, E. B. & Keating, J. P., 1996, Random-matrix theory and the Riemann zeros II: n-point correlations Nonlinearity 9, 911935.