EPFL Lectures on Quantum Physics III

Lectures: O. Yazyev
Exercises: J. Félisaz, X. Liu

Revised: 08.12.2025

Preface

These notes were originally written by M. Shaposhnikov, A. Shkerin, E. Tanin, and underwent a number of revisions since then. The notes include the discussion of classical limit of quantum mechanics, WKB approximation, scattering theory and relativistic quantum mechanics. The reader is assumed to be familiar with the material preceding the notes, including general principles of quantum theory, one-dimension motion of a quantum particle, harmonic oscillator.

Each lecture is supplemented with exercises. Advanced exercises are marked with an asterisk (*). The lectures are followed by the bibliography to which an interested reader is referred to for a more comprehensive study of particular topics. Attached in the end is the list of theory questions suggested to students at the end-term examination.

Contents

I From quantum to classical

Lecture 1 5

Lecture 2 14

II Semiclassical approximation

Lecture 3 22

Lecture 4 31

Lecture 5 41

III Scattering theory

Lecture 6 56

Lecture 7 61

Lecture 8 68

Lecture 9 74

Lecture 10 85

Lecture 11 89

IV Relativistic quantum mechanics

Lecture 12 102

Lecture 13 111

From quantum to classical

Lecture 1

> Classical limit of free particle and harmonic oscillator; definition of coherent states.

1.1 Quantum vs classical

It is a common practice to teach quantum physics by developing new ideas and notions from prerequisites of classical mechanics. In this approach, one starts with characteristics of a classical system, such as state (a pair of coordinate q and momentum p in phase space), observable (a function of q and p) and maps them to characteristics of a quantum system with quite different mathematical structure. For example, a quantum state is represented by a vector of unit norm in a complex vector space $\mathscr{H}$.[1] The counterpart of classical Hamiltonian and of any other observable is an hermitian operator acting in the space of quantum states, and so on; see Table 1.1 for a more complete list.

This way of introducing to quantum physics is well motivated by the correspondence principle claiming that, by applying a certain quantization procedure to some classical system, one arrives at the quantum system whose classical limit is the original system. The truth is that, however, quantum description of reality underlies the classical one, and it would be more in accordance with the logic of theoretical physics to come to the classical perspective starting from quantum principles and taking the limit $\hbar \to 0$ in an appropriate way. This would amount to reading Table 1.1 from right to left. In this lecture we start implementing this program by considering the two most standard examples of quantum systems — free particle and harmonic oscillator.

1.2 Free particle

A quantum free particle is described by the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m}\,, \tag{1.1}$$

which is obtained from the classical Hamiltonian by replacing the momentum p by the momentum operator $\hat{p}$. We would like to see how the behavior attributed to a classical point particle can emerge in this quantum system. In particular, in classical mechanics the point particle is characterized by definite values of its position and momentum. But, because of the uncertainty principle, it is clear

[1] More precisely, two unit vectors that are distinguished by phase still determine the same physical state. The name "ray" is adopted to refer to a vector defined "up to phase". One says, therefore, that physical states are represented by unit rays in Hilbert space.

Table 1.1: Ingredients for classical and quantum descriptions of physical systems.

	classical mechanics	quantum mechanics
state	(q,p)	unit-norm vector $\|\psi\rangle$ in Hilbert space $\mathscr{H}$
observable	c-number function of q and p	hermitian operator $\hat{O}$ acting in $\mathscr{H}$
time evolution	Newton's law $\vec{F}=m\ddot{\vec{x}}$	Schrodinger's equation $-\frac{\hbar}{i}\frac{\partial}{\partial t}\|\psi\rangle=\hat{H}\|\psi\rangle$
Hamiltonian	$H(q,p)$	$\hat{H}(\hat{q},\hat{p})$
measurement result	same as observable	$\frac{\langle\psi\|\hat{O}\psi\rangle}{\langle\psi\|\psi\rangle}$

that one cannot prepare a quantum state with this property. Indeed, consider the eigenstates of the Hamiltonian (1.1) in the x-representation,

$$\langle x|\psi_p\rangle\equiv\psi_p(x)=\frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}px}\ ,\quad \hat{H}\,|\psi_p\rangle=\frac{p^2}{2m}\,|\psi_p\rangle\ . \tag{1.2}$$

In $\psi_p(x)$ one recognizes familiar plane waves. The latter do have a definite momentum, but are completely delocalized in space, $|\psi_p(x)|^2=$const.[2] Hence, to build a state in which both the momentum and position operators have localized distributions, one should take a wave packet, that is, a certain linear combination of the plane waves (1.2). A natural choice is the state $|\psi_0\rangle$ described by the Gaussian distribution which we conveniently center at $x=0$,

$$\langle x|\psi_0\rangle\equiv\psi_0(x)=\frac{1}{\sqrt{\sigma}(2\pi)^{1/4}}e^{\frac{i}{\hbar}p_0x-\frac{x^2}{4\sigma^2}}\ . \tag{1.3}$$

Recall that the parameter $\sigma>0$ controls dispersion of the wave packet. The probability density to find a particle at position x is now normalized,

$$|\psi_0(x)|^2\sim e^{-\frac{x^2}{2\sigma^2}}\ ,\quad \int_{-\infty}^{\infty}dx\,|\psi_0(x)|^2=1\ . \tag{1.4}$$

Since the state $|\psi_0\rangle$ is composed of many eigenstates of the Hamiltonian, it is not characterized by a definite momentum. To find how the momentum is distributed in this state, we write it in the p-representation,[3]

$$\begin{aligned}\langle p|\psi_0\rangle&=\int_{-\infty}^{\infty}dx\,\langle p|x\rangle\,\langle x|\psi_0\rangle\\&=\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}dx\,e^{-\frac{i}{\hbar}px}\psi_0(x)=\sqrt{\frac{\sigma}{\hbar}}\left(\frac{2}{\pi}\right)^{1/4}e^{-\frac{\sigma^2}{\hbar^2}(p-p_0)^2}\ .\end{aligned} \tag{1.5}$$

We see that the momentum distribution is centered around p_0. Hence, a quantum free particle in the state $|\psi_0\rangle$ has the coordinate and momentum both localized. Quantitatively, computation of expectation values and mean squares of the operators $\hat{x}$ and $\hat{p}$ in this state gives

$$\begin{aligned}&\langle\hat{x}\rangle=0\ ,\quad \langle\hat{x}^2\rangle=\sigma^2\ ,\\&\langle\hat{p}\rangle=p_0\ ,\quad \langle(\hat{p}-p_0)^2\rangle=\frac{\hbar^2}{4\sigma^2}\ .\end{aligned} \tag{1.6}$$

[2] Strictly speaking, plane waves do not belong to the space of physical states. In particular, their probability density is not normalizable, see Addendum A for more details.

[3] See Addendum B for our convention about coefficients in Fourier transforms.

We conclude that, as long as resolution of our experimental tools is worse than σ in position and worse than $\hbar/2\sigma$ in momentum, the state $|\psi_0\rangle$ is seen to us as the state of classical particle with $x = 0$ and $p = p_0$.

The story does not end here as the state $|\psi_0\rangle$ evolves in time according to the Schrodinger equation and, hence, its position and momentum distributions can change. To track this change, one should solve the Cauchy problem

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \ , \quad |\psi(0)\rangle = |\psi_0\rangle \tag{1.7}$$

with $\hat{H}$ given in Eq. (1.1). The solution, in the x-representation, is

$$\begin{aligned}\psi(x,t) = \frac{\hbar\sqrt{\sigma}}{|\sigma(t)|(2\pi)^{1/4}}\exp\left[-\frac{i}{2}\arctan\left(\frac{\hbar t}{2m\sigma^2}\right) - \frac{i}{\hbar}\frac{p_0^2}{2m}t\right] \\ \times\exp\left[\frac{i}{\hbar}p_0 x - \frac{(x-p_0 t/m)^2}{4\sigma^2(t)}\right] \ ,\end{aligned} \tag{1.8}$$

where

$$\sigma^2(t) = \sigma^2 + i\frac{\hbar t}{2m} \ . \tag{1.9}$$

One can then work out that

$$\begin{aligned}&\langle\hat{x}\rangle = \frac{p_0 t}{m} \ , \quad \left\langle\left(\hat{x} - \frac{p_0 t}{m}\right)^2\right\rangle = \frac{|\sigma(t)|^4}{\sigma^2} = \sigma^2 + \frac{\hbar^2 t^2}{4m^2\sigma^2} \ , \\ &\langle\hat{p}\rangle = p_0 \ , \quad \langle(\hat{p}-p_0)^2\rangle = \frac{\hbar^2}{4\sigma^2} \ .\end{aligned} \tag{1.10}$$

From here we learn that, although the mean position and momentum of a quantum particle coincide with the position and momentum of a freely moving classical particle, the position uncertainty of the former grows with time,

$$\delta x \simeq |\sigma(t)| = \sigma\left(1 + \frac{\hbar^2 t^2}{4m^2\sigma^4}\right)^{1/2} \ , \tag{1.11}$$

and, given the fixed resolution of our experimental facility, the predictions based on classical mechanics will break down at some time. Thus, the wave packet is spreading as it travels freely along the x-axis. This limits the extent to which classical approximation of the quantum free particle system is valid. From Eqs. (1.10) one also sees that the momentum uncertainty δp does not grow with time.

1.3 Harmonic oscillator

Let us turn to another example of a quantum system for which analytical treatment is available. Consider harmonic oscillator with the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \ . \tag{1.12}$$

Recall that the coordinate and momentum operators $\hat{x}$ and $\hat{p}$ obey the commutation relation

$$[\hat{x},\hat{p}] = i\hbar \ . \tag{1.13}$$

It is convenient to introduce creation and annihilation operators

$$\begin{aligned}\hat{a} &= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\hat{x} + i\frac{1}{\sqrt{m\hbar\omega}}\hat{p}\right) ,\\ \hat{a}^\dagger &= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\hat{x} - i\frac{1}{\sqrt{m\hbar\omega}}\hat{p}\right) .\end{aligned} \tag{1.14}$$

From Eq. (1.13) one then obtains that

$$[\hat{a}, \hat{a}^\dagger] = 1 . \tag{1.15}$$

In terms of $\hat{a}$ and $\hat{a}^\dagger$, the Hamiltonian (1.12) is written as

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) . \tag{1.16}$$

As in the previous example, we start by determining eigenstates of this operator. One of the states, $|0\rangle$, is defined by the relation

$$\hat{a}\,|0\rangle = 0 \tag{1.17}$$

and determines the ground state of the oscillator. All other eigenstates $|n\rangle$, $n > 0$, are obtained by acting on $|0\rangle$ by the creation operator,

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n\,|0\rangle . \tag{1.18}$$

An eigenstate $|n\rangle$ obeys

$$\hat{H}\,|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle . \tag{1.19}$$

Again, we ask if the state $|n\rangle$ of the quantum harmonic oscillator exhibits properties of the classical counterpart. In classical mechanics, the coordinate and momentum of a particle moving in the harmonic potential evolve according to

$$\frac{dx(t)}{dt} = \frac{p(t)}{m} , \quad \frac{dp(t)}{dt} = -m\omega^2 x(t) . \tag{1.20}$$

From here we deduce the well-known oscillating behavior of, say, particle's position

$$x(t) = x_0 \sin(\omega t + \phi) , \tag{1.21}$$

where the parameters x_0 and ϕ are determined by initial conditions. This is in contrast with the eigenstates $|n\rangle$ for which

$$\langle n|\,\hat{x}\,|n\rangle = \langle n|\,\hat{p}\,|n\rangle = 0 . \tag{1.22}$$

Thus, the states $|n\rangle$ are not suitable for our purpose and one should look for appropriate linear combinations of them.

Recall that in the Heisenberg picture, the creation and annihilation operators evolve according to the Heisenberg equation,

$$\begin{aligned}-\frac{\hbar}{i}\frac{d\hat{a}}{dt} &= [\hat{a}, H] = \hbar\omega\hat{a} \quad \rightarrow \quad \hat{a}(t) = \hat{a}(0)e^{-i\omega t} ,\\ -\frac{\hbar}{i}\frac{d\hat{a}^\dagger}{dt} &= [\hat{a}^\dagger, H] = -\hbar\omega\hat{a}^\dagger \quad \rightarrow \quad \hat{a}^\dagger(t) = \hat{a}^\dagger(0)e^{+i\omega t} .\end{aligned} \tag{1.23}$$

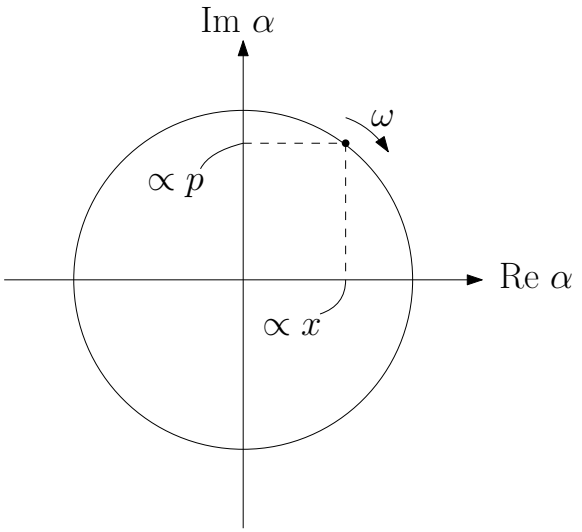


Figure 1.1: Time-evolution of α in the (Re α, Im α) plane.

From here one can also obtain the time-dependence of $\hat{x}$ and $\hat{p}$,

$$\begin{aligned}\hat{x}(t) &= \sqrt{\frac{\hbar}{2m\omega}}\left[\hat{a}(t)+\hat{a}^\dagger(t)\right] = \sqrt{\frac{\hbar}{2m\omega}}\left[\hat{a}(0)e^{-i\omega t}+\hat{a}^\dagger(0)e^{i\omega t}\right] ,\\ \hat{p}(t) &= \sqrt{\frac{m\hbar\omega}{2}}\frac{1}{i}\left[\hat{a}(t)+\hat{a}^\dagger(t)\right] = \sqrt{\frac{m\hbar\omega}{2}}\frac{1}{i}\left[\hat{a}(0)e^{-i\omega t}-\hat{a}^\dagger(0)e^{i\omega t}\right] .\end{aligned} \tag{1.24}$$

It is worth reminding that the Hamiltonian remains independent of time,

$$\hat{H}(t) = \hat{H}(0) = \hbar\omega\left[\hat{a}^\dagger(0)\hat{a}(0)+\frac{1}{2}\right] , \tag{1.25}$$

as follows directly from the Heisenberg equation and reflects the energy conservation law. The same is true for the commutator

$$[\hat{a}(t),\hat{a}^\dagger(t)] = 1 . \tag{1.26}$$

Consider now the *classical* observable $\alpha(t)$ defined according to (cf. Eq. (1.14))

$$\alpha(t) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x(t)+\frac{i}{\sqrt{m\omega\hbar}}p(t)\right) , \tag{1.27}$$

where $x(t)$ and $p(t)$ are solutions of Eqs. (1.20). Then,

$$\frac{d\alpha(t)}{dt} = -i\omega\alpha(t) , \quad \alpha(t) = \alpha_0 e^{-i\omega t} . \tag{1.28}$$

Hence, $\alpha(t)$ follows the same evolution in time as the annihilation operator in the Heisenberg picture $\hat{a}(t)$, see Fig. 1.1 for illustration. Furthermore, when expressed in terms of $\alpha(t)$ and $\alpha^*(t)$, the functions $x(t)$ and $p(t)$ become

$$\begin{aligned}x(t) &= \sqrt{\frac{\hbar}{2m\omega}}\left[\alpha_0 e^{-i\omega t}+\alpha_0^\dagger e^{i\omega t}\right] ,\\ \hat{p}(t) &= \sqrt{\frac{m\hbar\omega}{2}}\frac{1}{i}\left[\alpha_0 e^{-i\omega t}-\alpha_0^\dagger e^{i\omega t}\right] .\end{aligned} \tag{1.29}$$

Table 1.2: Comparison between quantum and classical descriptions of harmonic oscillator.

quantum	classical
$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$	$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$
$\hat{a} = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\hat{x} + i\frac{1}{\sqrt{m\hbar\omega}}\hat{p}\right)$	$\alpha = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x + i\frac{1}{\sqrt{m\hbar\omega}}p\right)$
$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$	$H = \hbar\omega\alpha^*\alpha$
$[\hat{a}, \hat{a}^\dagger] = 1$	$[\alpha, \alpha^*] = 0$
$\hat{a}(t) = \hat{a}(0)e^{-i\omega t}$	$\alpha(t) = \alpha_0 e^{-i\omega t}$
$\frac{d\langle\hat{x}\rangle}{dt} = \frac{\langle\hat{p}\rangle}{m}\,, \quad \frac{d\langle\hat{p}\rangle}{dt} = -m\omega^2\langle\hat{x}\rangle$	$\frac{dx}{dt} = \frac{p}{m}\,, \quad \frac{dp}{dt} = -m\omega^2 x$

We compare these expressions with the operator expressions (1.24) averaged with some state $|\psi_{\alpha_0}\rangle$:

$$\begin{aligned}\langle\hat{x}(t)\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\left[\langle\hat{a}(0)\rangle e^{-i\omega t} + \langle\hat{a}^\dagger(0)\rangle e^{i\omega t}\right]\,,\\ \langle\hat{p}(t)\rangle &= \sqrt{\frac{m\hbar\omega}{2}}\frac{1}{i}\left[\langle\hat{a}(0)\rangle e^{-i\omega t} - \langle\hat{a}^\dagger(0)\rangle e^{i\omega t}\right]\,.\end{aligned} \tag{1.30}$$

Eqs. (1.29) and (1.30) coincide upon identifying

$$\langle\psi_{\alpha_0}|\hat{a}|\psi_{\alpha_0}\rangle = \alpha_0\,. \tag{1.31}$$

Hence, the expectation values of $\hat{x}$ and $\hat{p}$ in the state $|\psi_{\alpha_0}\rangle$ satisfying Eq. (1.31) evolve as the coordinate and momentum of the classical oscillator.

Next, consider the energy of the classical oscillator written in terms of α_0,

$$H = \frac{p^2(0)}{2m} + \frac{1}{2}m\omega^2 x^2(0) = \hbar\omega|\alpha_0|^2\,. \tag{1.32}$$

If one requires the state $|\psi_{\alpha_0}\rangle$ to obey

$$\langle\psi_{\alpha_0}|\hat{a}^\dagger\hat{a}|\psi_{\alpha_0}\rangle = |\alpha_0|^2\,, \tag{1.33}$$

then the expectation value of the Hamiltonian (1.12) becomes

$$\langle\psi_{\alpha_0}|\hat{H}|\psi_{\alpha_0}\rangle = \hbar\omega\left(|\alpha_0|^2 + \frac{1}{2}\right)\,. \tag{1.34}$$

In the limit $|\alpha_0|^2 \gg 1$, Eqs. (1.32) and (1.34) coincide. Thus, we have the strong evidence that the states $|\psi_{\alpha_0}\rangle$ defined by Eqs. (1.31) and (1.33) exhibit behavior similar to that of the classical system. Such states are called *coherent* and we proceed to their study in the next lecture. Our current findings are summarized in Table 1.2.

Addendum A It is customary to identify states of a physical system with vectors or, more precisely, unit rays of some Hilbert space $\mathscr{H}$. The space is equipped with the scalar product $\langle\cdot|\cdot\rangle$ and is complete with respect to the norm topology defined by this product. However, such identification appears to fail when one attempts to deal with the states represented by "singular" functions. The examples are the continuous spectrum of eigenstates of the free

particle Hamiltonian, which in the momentum representation are all $\propto \delta(p)$. Such states — the plane waves — cannot be *real* physical states, i.e., the ones observed in experiment and with experimental tools of finite resolution. However, it is impossible to deny their value for calculations, as, for example, finding a Fourier transform of a given function amounts to decomposing it in a linear combination of the plane waves. This calls for a modification of the notion of space of physical states.

One of the possible ways to treat consistently "singular" objects is to use the "rigged" Hilbert space. It consists of the triplet

$$\mathscr{H} \subset \bar{\mathscr{H}} \subset \mathscr{H}^* \,. \tag{1.35}$$

Let us specify each of the components in this construction. One starts by defining a set of hermitian operators claimed to be observables in a given physical system. The space $\mathscr{H}$ is taken as an intersection of the domains of these observables. Hence, $\mathscr{H}$ is the physical space of states. It is equipped with the familiar scalar product $\langle\cdot|\cdot\rangle$ but, in general, not complete. The completion of $\mathscr{H}$ is denoted by $\bar{\mathscr{H}}$. The elements of $\bar{\mathscr{H}}$ can be thought of as antilinear functionals on $\mathscr{H}$. Indeed, for any $|\psi\rangle \in \bar{\mathscr{H}}$ one can define a functional

$$\Psi : \Psi(|\phi\rangle) = \langle\psi|\phi\rangle \;, \quad \phi \in \mathscr{H} \,. \tag{1.36}$$

The Hilbert space $\bar{\mathscr{H}}$ is in turn contained in the space $\mathscr{H}^*$ of all continuous antilinear functionals on $\mathscr{H}$. In particular, it includes the delta-functions discussed above.

The outlined construction allows to distinguish between the vectors of $\mathscr{H}$ representing the states that can be prepared in actual experiment and the vectors of $\mathscr{H}^*$ representing the states of an idealized system allowing for infinitely accurate measurements of continuous spectral parameters. It is also supported by, e.g., analysis of symmetries of quantum systems, see [1] for further discussion.

Addendum B Let us specify our normalization convention. Given a function $\psi(x)$, we define its Fourier transform as

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx\, \psi(x) e^{-\frac{i}{\hbar}px} \,. \tag{1.37}$$

This is equivalent to setting

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}px} \tag{1.38}$$

provided that

$$\int_{-\infty}^{\infty} dx\, |x\rangle\langle x| = 1 \,. \tag{1.39}$$

From Eq. (1.38) it follows that

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}px} \,, \tag{1.40}$$

hence, the inverse Fourier transform is given by

$$\tilde{\psi}(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp\, \psi(p) e^{\frac{i}{\hbar}px} \tag{1.41}$$

given that

$$\int_{-\infty}^{\infty} dp\, |p\rangle\langle p| = 1 \,. \tag{1.42}$$

Finally, from Eqs. (1.38)—(1.40) and (1.42) we obtain

$$\int_{-\infty}^{\infty} dp\, e^{\frac{i}{\hbar}pz} = 2\pi\hbar\delta(z) \,, \tag{1.43}$$

where the delta-function is defined according to

$$\int_{-\infty}^{\infty} dz\, \delta(z) = 1 \,. \tag{1.44}$$

▪ **Exercise 1.1 — Gaussian Integrals.** In section 1.2 we encountered Gaussian functions. Integrals of these functions are of particular importance in physics, and we will meet them multiple times throughout the notes. Calculate

$$I_1 = \int_{-\infty}^{\infty} dx\, e^{-\frac{x^2}{2}}\,, \quad I_2 = \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}ax^2+bx}\,, \quad I_3 = \int_{-\infty}^{\infty} dx\, x^2\, e^{-\frac{x^2}{2}}\,, \tag{1.45}$$

where a is real and positive and b is complex. ▪

▪ **Exercise 1.2 — A Gaussian packet.** Here we study in detail evolution of the Gaussian state of free particle considered in section 1.2. Consider the following Cauchy problem,

$$-\frac{\hbar}{i}\frac{d\psi(p,t)}{dt} = H\psi(p,t)\,, \quad H = \frac{p^2}{2m}\,, \quad \psi(p,0) = \frac{A}{(2\pi)^{1/4}} e^{-\frac{\sigma^2}{\hbar^2}(p-p_0)^2}\,, \tag{1.46}$$

where

$$\psi(p,0) = \langle p|\psi\rangle\,, \quad \psi(p,t) = \langle p|\psi(t)\rangle\,, \tag{1.47}$$

and $|\psi\rangle$ is a unit-norm Gaussian state.

1. Determine the normalization constant A.
2. Find the Fourier image $\psi(x,0)$ of $\psi(p,0)$. Compute the dispersions $\Delta\hat{x}$ and $\Delta\hat{p}$ of the operators $\hat{x}$ and $\hat{p}$ in the state $|\psi\rangle$.
3. Find $\psi(p,t)$ and $\psi(x,t)$. Write the expressions for the dispersions $\Delta\hat{x}$, $\Delta\hat{p}$ in the state $|\psi(t)\rangle$ and describe their time-dependence. What can one say about the quantity $\Delta\hat{x}\cdot\Delta\hat{p}$ at $t=0$ and $t>0$?

▪

▪ **Exercise 1.3 — Quantum fluctuations.** Consider a hill with a flat top of length $l = 1\ cm$ at the center of which an object of size smaller than l and mass $m = 1\ g$ is placed.

1. Treating the object as a Gaussian packet, find how long it can stay on the top before quantum fluctuations drive it out. Assume that there is no interaction between the object and the hill.
2. Compute this time in the case when the dispersion of the object is $\sigma = 10^{-9}\ cm$.

▪

▪ **Exercise 1.4 — Harmonic oscillator.** Let $\hat{H}$ and H be the Hamiltonians of quantum and classical harmonic oscillators respectively, $\hat{a}$, $\hat{a}^\dagger$ and $\hat{a}(t)$, $\hat{a}^\dagger(t)$ be annihilation and creation operators in the Schroedinger and Heisenberg pictures respectively.

1. Calculate $[\hat{a},\hat{H}]$, $[\hat{a}^\dagger,\hat{H}]$, and $[\hat{a}(t),\hat{a}^\dagger(t)]$.
2. Calculate the expression for H in terms of classical variables $\alpha(t)$ and $\alpha^*(t)$ with
   $\alpha(t) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x(t) + i\sqrt{\frac{1}{\hbar m\omega}}p(t)\right)$,
   where $x(t)$, $p(t)$ satisfy Eqs. (1.20).

▪

▪ **Exercise 1.5 — Gaussian integrals in more dimensions.** Consider an $N\times N$ real positive definite symmetric matrix A and two N-dimensional vectors x and B.

1. Show that

$$\int_{-\infty}^{\infty}\ldots\int_{-\infty}^{\infty} dx_1\ldots dx_N\, e^{-\frac{1}{2}x^tAx+B^tx} = \frac{(2\pi)^{N/2}}{\sqrt{\det A}}\exp\left(\frac{1}{2}B^tA^{-1}B\right)\,. \tag{1.48}$$

   Note: The result also holds for a complex symmetric A with a positive definite $\mathrm{Re}\,A$ and an arbitrary complex vector B (no conjugation!). The generalization of these integrals to infinite dimensional space is the *path integral* studied in the next lectures.

2. Consider the "gaussian average" (or *correlator*) defined as

$$\langle x_{i_1} x_{i_2} \ldots x_{i_p} \rangle = \frac{\int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} dx_1 \ldots dx_N \, e^{-\frac{1}{2} x^t A x} x_{i_1} \ldots x_{i_p}}{\int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} dx_1 \ldots dx_N \, e^{-\frac{1}{2} x^t A x}} \, . \tag{1.49}$$

Show that

$$\langle x_{i_1} x_{i_2} \rangle = \left(A^{-1}\right)_{i_1 i_2} \, ,$$

$$\langle x_{i_1} x_{i_2} x_{i_3} x_{i_4} \rangle = \langle x_{i_1} x_{i_2} \rangle \langle x_{i_3} x_{i_4} \rangle + \langle x_{i_1} x_{i_3} \rangle \langle x_{i_2} x_{i_4} \rangle + \langle x_{i_1} x_{i_4} \rangle \langle x_{i_2} x_{i_3} \rangle \, , \tag{1.50}$$

$$\langle x_{i_1} x_{i_2} \ldots x_{i_k} \rangle = 0 \, , \quad \text{if } \; k \; \text{ is odd.}$$

Note: The formula (1.50) is an example of the so-called *Wick theorem*: the expectation value can be obtained by summing over all possible pairwise contractions. Note also that inserting into the exponent in (1.49) higher order terms in x would break this nice relation between the different correlators.

▪

Lecture 2

> Coherent states in terms of eigenstates of the harmonic oscillator; properties of coherent states; coherent state wavefunction in the x-representation.

2.1 Coherent states in terms of eigenstates of the harmonic oscillator

This lecture is dedicated to the coherent states $|\psi_\alpha\rangle$ of the harmonic oscillator, introduced before in Eqs. (1.31) and (1.33). Following the logic of the previous lecture, we would like to see how close they are in their behavior to the classical oscillator.

We start by expanding $|\psi_\alpha\rangle$ in a linear combination of the eigenstates $|n\rangle$ of the Hamiltonian (1.12). Consider the expression

$$\langle\psi_\alpha|\,(\hat{a}-\alpha)^\dagger(\hat{a}-\alpha)\,|\psi_\alpha\rangle = \langle\psi_\alpha|\left(\hat{a}^\dagger\hat{a}-\alpha\hat{a}^\dagger-\alpha^*\hat{a}+|\alpha|^2\right)|\psi_\alpha\rangle\ . \tag{2.1}$$

By using Eqs. (1.31) and (1.33), it reduces to

$$\langle\psi_\alpha|\,(\hat{a}-\alpha)^\dagger(\hat{a}-\alpha)\,|\psi_\alpha\rangle = |\alpha|^2-\alpha\alpha^*-\alpha^*\alpha+|\alpha|^2 = 0\,. \tag{2.2}$$

This means that

$$(\hat{a}-\alpha)|\psi_\alpha\rangle = 0\,, \tag{2.3}$$

or

$$\hat{a}\,|\psi_\alpha\rangle = \alpha\,|\psi_\alpha\rangle\ . \tag{2.4}$$

We have obtained that $|\psi_\alpha\rangle$ is, in fact, an eigenstate of the annihilation operator, with the complex eigenvalue α. Since the operator $\hat{a}$ is not degenerate, from Eq. (2.4) it follows that for a fixed α there is a unique coherent state $|\psi\rangle$ such that $\hat{a}\,|\psi\rangle = \alpha\,|\psi\rangle$. Because of this, from now one we will conveniently denote the coherent states as $|\alpha\rangle$.

Since the energy states $|n\rangle$ form a basis in the Hilbert space of states of the harmonic oscillator, one can expand

$$|\alpha\rangle = \sum_{n=0}^{\infty} C_n\,|n\rangle\ . \tag{2.5}$$

Our goal is to find the coefficients $C_n = C_n(\alpha)$ in this expansion. To this end, we act by $\hat{a}$ on both sides of Eq. (2.5) and use Eq. (2.4):

$$\begin{aligned} \hat{a}\sum_{n=0}^{\infty} C_n |n\rangle &= \alpha \sum_{n=0}^{\infty} C_n |n\rangle \ , \\ \sum_{n=1}^{\infty} C_n \sqrt{n}\,|n-1\rangle &= \alpha \sum_{n=0}^{\infty} C_n |n\rangle \ , \\ \sum_{n=0}^{\infty} C_{n+1} \sqrt{n+1}\,|n\rangle &= \alpha \sum_{n=0}^{\infty} C_n |n\rangle \ , \end{aligned} \tag{2.6}$$

It, therefore, follows that

$$C_{n+1} = \frac{\alpha}{\sqrt{n+1}} C_n \ . \tag{2.7}$$

It is easy to see that this leads to

$$C_n = \frac{\alpha^n}{\sqrt{n!}} C_0 \ . \tag{2.8}$$

Plugging Eq. (2.8) back to Eq. (2.5) gives

$$|\alpha\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} C_0 |n\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} C_0 \left[\frac{\left(\hat{a}^\dagger\right)^n}{\sqrt{n!}} |0\rangle \right] = C_0\, e^{\alpha \hat{a}^\dagger} |0\rangle \ . \tag{2.9}$$

Finally, C_0 can be found from the normalization condition

$$\begin{aligned} 1 = \langle \alpha |\, \alpha \rangle &= \langle \alpha | C_0\, e^{\alpha \hat{a}^\dagger} |0\rangle \\ &= C_0\, e^{|\alpha|^2} \langle \alpha |\, 0\rangle = |C_0|^2\, e^{|\alpha|^2} \ . \end{aligned} \tag{2.10}$$

Then,

$$C_0 = \exp\left(-\frac{1}{2}|\alpha|^2 \right) \ , \tag{2.11}$$

where without loss of generality we set the phase of C_0 to zero. Thus,

$$|\alpha\rangle = \exp\left(-\frac{1}{2}|\alpha|^2 + \alpha \hat{a}^\dagger \right) |0\rangle \ . \tag{2.12}$$

2.2 Properties of coherent states

As we saw in lecture 1, the expectation values of position, momentum and Hamiltonian in a coherent state coincide with the corresponding classical quantities in the limit $|\alpha| \gg 1$. We now want to look in more detail at coordinate and energy wavefunctions of the coherent states.

First, we compute the energy distribution $\mathscr{P}_n = |\langle n|\alpha\rangle|^2$. It gives a probability for the state $|\alpha\rangle$ to have an energy of the n'th level of the harmonic oscillator. Using Eq. (2.5), we find

$$\mathscr{P}_n = |C_n|^2 = e^{-|\alpha|^2} \frac{|\alpha|^{2n}}{n!} \ . \tag{2.13}$$

Since we are interested in the regimes of large $|\alpha|$ and, presumably, large n, Stirling's approximation of the factorial is applicable,

$$n! \sim n^n e^{-n} \sqrt{2\pi n} \ , \quad n \to \infty \ . \tag{2.14}$$

Eq. (2.13) becomes

$$\mathscr{P}_n \approx \frac{1}{\sqrt{2\pi n}}\, e^{S(n)}\,, \tag{2.15}$$

where

$$S(n) = -n\log n + n + 2n\log|\alpha| - |\alpha|^2\,. \tag{2.16}$$

The probability distribution is concentrated around the maximum of the function $S(n)$. At this maximum

$$\frac{\partial}{\partial n}S(n) = -\log n - 1 + 1 + 2\log|\alpha| = 0\,, \tag{2.17}$$

which happens when

$$n = \bar{n} \equiv |\alpha|^2\,. \tag{2.18}$$

This confirms that $|\alpha|^2$ determines the mean energy (or the mean number of particles) in the state $|\alpha\rangle$. Computing the second derivative gives

$$\frac{\partial^2}{\partial n^2}S(n)\bigg|_{n=\bar{n}} = -\frac{1}{\bar{n}} = -\frac{1}{|\alpha|^2}\,. \tag{2.19}$$

Hence, $n=\bar{n}$ is indeed the maximum point of $S(n)$. Near this point, $\mathscr{P}_n$ can be approximated as

$$\begin{aligned}\mathscr{P}_n &\approx \frac{1}{\sqrt{2\pi\bar{n}}}\exp\left[S(\bar{n}) + \frac{1}{2}\,\frac{\partial^2}{\partial n^2}S(n)\bigg|_{n=\bar{n}}(n-\bar{n})^2\right] \\ &= \frac{1}{\sqrt{2\pi|\alpha|^2}}\exp\left[-\frac{\left(n-|\alpha|^2\right)^2}{2|\alpha|^2}\right]\,.\end{aligned} \tag{2.20}$$

This is the Gaussian distribution with the peak at $n=|\alpha|^2$ and with the width

$$\Delta n \sim |\alpha| \ll |\alpha|^2\,, \quad |\alpha| \gg 1\,. \tag{2.21}$$

We conclude that in the limit $|\alpha| \gg 1$ the energy of the coherent state $|\alpha\rangle$ is well determined.

Second, let us see how the coordinate and momentum operators are distributed in the coherent states. From Eqs. (1.24) and (1.31), (1.33) we obtain

$$\begin{aligned}&\langle\alpha|\,\hat{x}\,|\alpha\rangle = \sqrt{\frac{2\hbar}{m\omega}}\,\mathrm{Re}\,\alpha\,, && \langle\alpha|\,\hat{p}\,|\alpha\rangle = \sqrt{2m\hbar\omega}\,\mathrm{Im}\,\alpha\,, \\ &\langle\alpha|\,\hat{x}^2\,|\alpha\rangle = \frac{\hbar}{2m\omega}\left[4\,(\mathrm{Re}\,\alpha)^2 + 1\right]\,, && \langle\alpha|\,\hat{p}^2\,|\alpha\rangle = \frac{m\hbar\omega}{2}\left[4\,(\mathrm{Im}\,\alpha)^2 + 1\right]\,.\end{aligned} \tag{2.22}$$

From here, one can compute the position and momentum uncertainties,

$$\begin{aligned}\Delta\hat{x} &= \sqrt{\langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2} = \sqrt{\frac{\hbar}{2m\omega}}\,, \\ \Delta\hat{p} &= \sqrt{\langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2} = \sqrt{\frac{m\hbar\omega}{2}}\,.\end{aligned} \tag{2.23}$$

Multiplying the two, one arrives at

$$\Delta\hat{x}\cdot\Delta\hat{p} = \frac{\hbar}{2}\,. \tag{2.24}$$

Thus, the coherent states minimize the uncertainty relation. Furthermore, since the r.h.s. of Eq. (2.24) shows no dependence on α, this result remains valid at any time. As for the expectation values of $\hat{x}$ and $\hat{p}$, according to Eq. (2.22), they follow the classical oscillation laws. Overall, we see that the coherent states serve as a very good approximation to the classical harmonic oscillator.

2.3 Coherent state wavefunction in the x-representation

The goal of this section is to compute explicitly the coordinate wavefunction of a coherent state, $\psi_\alpha(x) = \langle x|\,\alpha\rangle$. To this end, it proves useful to define the following operator,

$$\hat{D}(\alpha) = \exp\left(\alpha\hat{a}^\dagger - \alpha^*\hat{a}\right) \tag{2.25}$$

with α a complex number. One can check that $\hat{D}$ is unitary,

$$\hat{D}^\dagger\hat{D} = \hat{D}\hat{D}^\dagger = 1\,. \tag{2.26}$$

Using Glauber's formula,[1]

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}}e^{\frac{1}{2}[\hat{A},\hat{B}]}\,, \tag{2.27}$$

which is valid as long as $[\hat{A},[\hat{A},\hat{B}]] = [\hat{B},[\hat{A},\hat{B}]] = 0$, one can write $\hat{D}$ in the form

$$\hat{D}(\alpha) = e^{\alpha\hat{a}^\dagger}e^{-\alpha^*\hat{a}}e^{\frac{1}{2}[\alpha\hat{a}^\dagger,\alpha^*\hat{a}]} = e^{-\frac{1}{2}|\alpha|^2}e^{\alpha\hat{a}^\dagger}e^{-\alpha^*\hat{a}}\,. \tag{2.28}$$

Acting by it on the ground state $|0\rangle$ of the oscillator, we find

$$\hat{D}(\alpha)\,|0\rangle = e^{-\frac{1}{2}|\alpha|^2}e^{\alpha\hat{a}^\dagger}e^{-\alpha^*\hat{a}}\,|0\rangle = \exp\left(-\frac{1}{2}|\alpha|^2 + \alpha\hat{a}^\dagger\right)|0\rangle = |\alpha\rangle\,, \tag{2.29}$$

where in the first and second equalities we have used $e^{-\alpha^*\hat{a}}\,|0\rangle = |0\rangle$ and Eq. (2.12) respectively. We see that the operator $\hat{D}(\alpha)$ converts the ground state $|0\rangle$ into the coherent state $|\alpha\rangle$.

One can now proceed to evaluating $\psi_\alpha(x)$. Multiplying Eq. (2.29) by $\langle x|$, one has

$$\begin{aligned}
\psi_\alpha(x) &= \left\langle x|\hat{D}(\alpha)|0\right\rangle \\
&= \langle x|\exp\left(\alpha\hat{a}^\dagger - \alpha^*\hat{a}\right)|0\rangle \\
&= \langle x|\exp\left(\frac{i}{\hbar}\langle\hat{p}\rangle\hat{x} - \frac{i}{\hbar}\hat{p}\,\langle\hat{x}\rangle\right)|0\rangle \\
&= \exp\left(i\theta_\alpha\right)\langle x|\exp\left(\frac{i}{\hbar}\langle\hat{p}\rangle\hat{x}\right)\exp\left(-\frac{i}{\hbar}\hat{p}\,\langle\hat{x}\rangle\right)|0\rangle \\
&= \exp\left(\frac{i}{\hbar}\langle\hat{p}\rangle x - i\theta_\alpha\right)\langle x - \langle\hat{x}\rangle\,|0\rangle \\
&= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(\frac{i}{\hbar}\langle\hat{p}\rangle x - i\theta_\alpha\right)\exp\left(-\frac{x^2}{4(\Delta\hat{x})^2}\right)\,,
\end{aligned} \tag{2.30}$$

where

$$\theta_\alpha = \frac{(\alpha^*)^2 - \alpha^2}{4i} \tag{2.31}$$

and all expectations are taken with $|\alpha\rangle$. In going from the second to third line, we simply expressed α, α^*, $\hat{a}$, $\hat{a}^\dagger$ in terms of $\langle\hat{x}\rangle$, $\hat{x}$, $\langle\hat{p}\rangle$, and $\hat{p}$; from the third to fourth line we employed Glauber's formula (2.27); from the fourth to fifth line we used the fact that $\exp\left(-\frac{i}{\hbar}\hat{p}\,\langle\hat{x}\rangle\right)$ is a generator of translation by $\langle\hat{x}\rangle$. Finally, in the last step we substituted the explicit form of the ground state wavefunction of harmonic oscillator,

$$\langle x|0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{(x-\langle\hat{x}\rangle)^2}{4(\Delta\hat{x})^2}\right)\,,\quad \Delta\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\,. \tag{2.32}$$

[1] For its proof, see addendum A.

The same derivation can now be repeated to reveal the time dependence of the coherent state wavefunction, $\psi_\alpha(x,t) = \langle x|\alpha(t)\rangle$. It simply amounts to taking a bracket with $|\alpha(t)\rangle$ instead of $|\alpha\rangle$ in the last line of Eq. (2.30) and to multiplying the result by the factor $\exp(-i\omega t/2)$ coming from the time evolution of the ground state $|0\rangle$. The conclusion is that the coherent wave packet moves without the distortion in time (hence the name) and the position of the center of the packet follows the classical equation of motion of the harmonic oscillator.

Addendum A Let us prove Glauber's formula: if A and B are operators such that (we omit the hats below)

$$[A,[A,B]] = 0\,, \quad [B,[A,B]] = 0\,, \tag{2.33}$$

then

$$e^A e^B = e^{\frac{1}{2}[A,B]} e^{A+B}\,. \tag{2.34}$$

Consider an operator function

$$F(t) = e^{tA} e^{tB} e^{-t(A+B)}\,. \tag{2.35}$$

Differentiating it gives

$$\begin{aligned} \frac{dF(t)}{dt} &= Ae^{tA}e^{tB}e^{-t(A+B)} + e^{tA}Be^{tB}e^{-t(A+B)} - e^{tA}e^{tB}(A+B)e^{-t(A+B)} \\ &= e^{tA}[A,e^{tB}]e^{-t(A+B)}\,. \end{aligned} \tag{2.36}$$

Now, consider the commutator $[A,B^n]$. By virtue of the second of Eqs. (2.33), we have

$$[A,B^n] = [A,B^{n-1}B] = [A,B^{n-1}]B + B^{n-1}[A,B] = [A,B^{n-1}]B + [A,B]B^{n-1}\,. \tag{2.37}$$

We expressed the commutator of n'th degree in B in terms of the commutator of $(n-1)$'th degree. Repeating this $n-1$ times leads to

$$[A,B^n] = [A,B]B^{n-1} + (n-1)[A,B]B^{n-1} = n[A,B]B^{n-1}\,. \tag{2.38}$$

Using Eq. (2.38), one can rewrite the commutator $[A,e^{tB}]$ in Eq. (2.36),

$$\begin{aligned} [A,e^{tB}] = \sum_{n=1}^{\infty} \frac{1}{n!}[A,(tB)^n] &= \sum_{n=1}^{\infty} \frac{1}{n!} nt^n [A,B]B^{n-1} \\ &= t[A,B]\sum_{n=1}^{\infty} \frac{t^{n-1}B^{n-1}}{(n-1)!} = t[A,B]e^{tB}\,. \end{aligned} \tag{2.39}$$

Hence,

$$\frac{dF(t)}{dt} = e^{tA}t[A,B]e^{tB}e^{-t(A+B)} = t[A,B]F(t)\,, \tag{2.40}$$

where in the second equality we used the first of Eqs. (2.33). Integrating this, one obtains

$$F(t) = e^{\frac{t^2}{2}[A,B]}\,. \tag{2.41}$$

Taking $t=1$, we arrive at Eq. (2.34).

Glauber's formula generalizes to the case when no commutation relations (2.33) are assumed:

$$e^{A+B} = e^A e^B e^{Z_2} e^{Z_3} e^{Z_4} \ldots\,, \tag{2.42}$$

where

$$\begin{aligned} Z_2 &= \frac{1}{2}[B,A] \\ Z_3 &= -\frac{1}{3}[B,[B,A]] - \frac{1}{6}[A,[B,A]] \\ Z_4 &= \frac{1}{8}\left([[[B,A],B],B] + [[[B,A],A],B]\right) + \frac{1}{24}[[[B,A],A],A] \\ &\vdots \end{aligned} \tag{2.43}$$

This is the Zassenhaus formula. We will not use it in these lectures, but we will make use of the fact that the terms Z_n, $n \geqslant 2$, all include ever-increasing towers of commutators of A and B. This is simply deduced by reconsidering Eqs. (2.37), (2.39) and (2.40) in the case when Eqs. (2.33) do not hold.

▪ **Exercise 2.1 — Classical limit of harmonic oscillator.** Let $\langle \hat{A} \rangle$ denote the matrix element $\langle \alpha | \hat{A} | \alpha \rangle$, where $|\alpha\rangle$ is a coherent state of the harmonic oscillator. Denote also $\hat{N} = \hat{a}^\dagger \hat{a}$.

1. Compute $\langle \hat{H} \rangle$, $\Delta\hat{H}$, $\langle \hat{N} \rangle$, $\Delta\hat{N}$, $\langle \hat{x} \rangle$, $\Delta\hat{x}$, $\langle \hat{p} \rangle$, $\Delta\hat{p}$. What is the product $\Delta\hat{x} \cdot \Delta\hat{p}$? Write the validity conditions for the classical treatment of the oscillator. What do they impose on $|\alpha|$?
2. As an application, consider a classical pendulum of length $l = 0.1\ m$ and mass $m = 1\ kg$ placed in the gravitational field of the Earth and performing a periodic motion with the amplitude $x_M = 1\ cm$. Let us treat it as a coherent state $|\alpha\rangle$ for some α. Find the numerical values of $|\alpha|$, $\Delta\hat{x}$, $\Delta\hat{p}$, $\Delta\hat{H}$ and $\langle \hat{H} \rangle$ and check the validity of the classical description.

▪

▪ **Exercise 2.2 — Properties of the displacement operator.** Let $\hat{D}(\alpha)$ be an operator generating the coherent state $|\alpha\rangle$ from the ground state $|0\rangle$ of the harmonic oscillator, see Eqs. (2.25) and (2.29). Prove that

- $\hat{D}$ is unitary;
- $\hat{D}^\dagger(\alpha)\hat{a}\hat{D}(\alpha) = \hat{a} + \alpha \cdot \hat{1}$;
- $\hat{D}(\alpha+\beta) = \hat{D}(\alpha)\hat{D}(\beta)e^{-i\,\mathrm{Im}(\alpha\beta^*)}$;
- $\hat{D}(\alpha)\hat{D}(\beta) = e^{2i\,\mathrm{Im}(\alpha\beta^*)}\hat{D}(\beta)\hat{D}(\alpha)$.

▪

▪ **Exercise 2.3 — Completeness of coherent states.** We know that the eigenstates $|n\rangle$ of harmonic oscillator constitute an orthogonal basis in the Hilbert space $\mathscr{H}$. We say that the basis forms a *complete* set of states if an arbitrary state from $\mathscr{H}$ can be decomposed into a linear combination of the basis states. The completeness can also be expressed as a resolution of identity:

$$\sum_n |n\rangle\langle n| = 1 \,. \tag{2.44}$$

Is the set of coherent states $\mathscr{A} = \{|\alpha\rangle,\ \alpha \in \mathbb{C}\}$ also complete? Intuitively, we expect an affirmative answer to this question, simply because $\mathscr{A}$ is much wider than the discrete set of eigenvalues $\{|n\rangle,\ n = 0,1,2,...\}$. In fact, the set $\mathscr{A}$ is *overcomplete*, that is, not all of $|\alpha\rangle$ are linearly independent of each other. This exercise is suggested to demonstrate the completeness and overcompleteness of $\mathscr{A}$.

1. Show first that

$$\int d^2\alpha e^{-|\alpha|^2}\alpha^{*n}\alpha^m = \pi n!\delta_{nm} \,, \tag{2.45}$$

where the integration measure $d^2\alpha$ is defined as

$$d^2\alpha = d\mathrm{Re}\,\alpha\, d\mathrm{Im}\,\alpha\ . \tag{2.46}$$

Hint: Use polar coordinates.

2. Now prove the completeness by showing that

$$\int \frac{d^2\alpha}{\pi}|\alpha\rangle\langle\alpha| = 1\ . \tag{2.47}$$

3. Compute the scalar product $\langle\alpha|\alpha'\rangle$ and the transition probability $|\langle\alpha|\alpha'\rangle|^2$. Are the coherent states orthogonal to each other?
4. Using the last result, show that any coherent state can be expanded through other coherent states. Hence, the system $\mathscr{A}$ is indeed overcomplete.
5. As another way to prove overcompleteness, find a real function $f(|\alpha|)$ such that

$$\int d^2\alpha f(|\alpha|)|\alpha\rangle = 0\ . \tag{2.48}$$

▪

▪ **Exercise 2.4 — Squeezed states.** We now know that the coherent states minimize the uncertainty relation at any time. Are there other states whose behavior is close to that of the classical oscillator? Consider the following state $|\Psi_\lambda\rangle$ (at $t = 0$):

$$|\Psi_\lambda\rangle \text{ is such that } \langle x|\Psi_\lambda\rangle \equiv \Psi_\lambda(x) = C\Psi_\alpha(\lambda x)\ , \tag{2.49}$$

with λ some real constant, C a normalization factor and $|\Psi_\alpha\rangle \equiv |\alpha\rangle$ a coherent state of harmonic oscillator. The states of the form (2.49) are called *squeezed* states. The name comes from the fact that for such states the dispersions of the coordinate and momentum operators can be less than those for the ground state of harmonic oscillator. Given below is a chain of exercises aiming to unveil some properties of squeezed states.

1. Determine the normalization factor C.
2. For the state $|\Psi_\lambda\rangle$ find $\langle\hat{x}\rangle$, $\langle\hat{p}\rangle$, $\Delta\hat{x}$, $\Delta\hat{p}$. What is the value of $\Delta\hat{x}\cdot\Delta\hat{p}$?
3. Find a *unitary* operator $\hat{S}_\lambda$ whose action on $|\Psi_\alpha\rangle$ gives $|\Psi_\lambda\rangle$. *Hint:* Recall that the coordinate shift $\Psi(x) \Rightarrow \Psi(x+a)$ can be achieved by the action of a translation operator of the form $\hat{T}(a) = e^{\frac{i}{\hbar}\hat{P}\cdot a}$.
4. Show that the time-evolved state $|\Psi_\lambda(t)\rangle$ can be expressed as

$$|\Psi_\lambda(t)\rangle = \hat{S}_\lambda(-t)|\Psi_\alpha(t)\rangle\ , \tag{2.50}$$

where $\hat{S}_\lambda(-t)$ is the operator $\hat{S}_\lambda$ in the Heisenberg picture.

5. Express $\hat{S}_\lambda(-t)$ in terms of the creation and annihilation operators $\hat{a}$, $\hat{a}^\dagger$ of the harmonic oscillator.
6. Now compute the expressions $\hat{S}^\dagger_\lambda(-t)\,\hat{a}\,\hat{S}_\lambda(-t)$ and $\hat{S}^\dagger_\lambda(-t)\,\hat{a}^\dagger\,\hat{S}_\lambda(-t)$.
7. Using the results of the p. 6, find the dispersions $\Delta\hat{x}$ and $\Delta\hat{p}$ for the state $|\Psi_\lambda(t)\rangle$ at $t \geqslant 0$. Check that they match with the results of the p. 2 at $t = 0$. Describe the time evolution of $\Delta\hat{x}$ and $\Delta\hat{p}$. Does the state $|\Psi_\lambda(t)\rangle$ minimize the uncertainty relation for the pair of operators $\hat{x}$, $\hat{p}$ at arbitrary $t > 0$? At some specific $t > 0$?
8. Find a time-dependent canonical transformation of the operators $\hat{x}$ and $\hat{p}$ such that the transformed operators $\hat{x}'$, $\hat{p}'$ minimize the uncertainty relation in the state $|\Psi_\lambda(t)\rangle$ at any $t > 0$.

▪

II

Semiclassical approximation

Lecture 3

> Semiclassical expansion; semiclassical wavefunction in the physical optics approximation; validity of the semiclassical approximation; turning points.

3.1 Semiclassical expansion

According to the correspondence principle, a quantum system must possess a classical limit in which dispersions of physical observables are negligible when considering dynamics of their expectation values. As we saw in the previous lectures, normally this limit corresponds to large quantum numbers $n \gg 1$, where n can denote, for example, a number of particles populating an energy level of the harmonic oscillator. We employed the path integral representation of the quantum evolution amplitude to show that, in fact, the classical limit of the dynamics of a quantum system matches the geometrical optics limit of wave mechanics. Indeed, in the latter limit effects of light interference are not important and the description of light in terms of corpuscules becomes legitimate. Neglecting interference, in turn, amounts to neglecting fluctuations around a stationary path in the functional integral (**??**).

As was discussed before, corrections to the leading-order saddle-point approximation of the evolution amplitude come as a series with respect to $\hbar$. As soon as one leaves aside the question of convergence of such series, this goes in accordance with the expectation that sending $\hbar$ to zero in an appropriate way yields the classical limit of a quantum system. Another argument supporting this expectation comes from the uncertainty relation: for two observables $\hat{A}$ and $\hat{B}$,

$$\Delta\hat{A} \cdot \Delta\hat{B} \geqslant \frac{\hbar}{2} |[\hat{A}, \hat{B}]| \,. \tag{3.1}$$

If $\hbar \to 0$, the fluctuations of the observables become unimportant. Of course, Eq. (3.1) provides a necessary, but not sufficient condition of validity of the classical treatment. These arguments motivate us to inspect the limit of "small $\hbar$" more closely. More precisely, since $\hbar$ is a dimensional parameter, it is a ratio of it to some quantity of the dimension of action (joule·s), which should be taken as a small parameter. Given the small parameter, one can build a perturbation theory whose zero order corresponds to the classical limit, and higher orders — to quantum corrections to that limit. This method of perturbative computation of quantum corrections is called WKB method, named after its proponents: Wentzel, Kramers, and Brillouin.

We start with writing the wave function in the x-representation $\psi(x,t)$ as follows,

$$\psi(x,t) = e^{\frac{i}{\hbar} S(x,t)} \,, \tag{3.2}$$

where $S(x,t)$ is, in general, a complex-valued function of x and t. Substituting Eq. (3.2) into the Schroedinger equation,

$$-\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi\,, \tag{3.3}$$

one obtains

$$-\frac{\partial S}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 S}{\partial x^2} + \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + V(x)\,. \tag{3.4}$$

If $\hbar$ is taken to be zero, the first term in the r.h.s. of the equation above disappears, and the Hamilton-Jacobi equation for the action of classical particle is reproduced. Thus, we have arrived at the classical limit of the Schroedinger equation. The complex phase $S/\hbar$ satisfies Fermat's principle.

From now on, we will consider stationary states for which

$$\psi(x,t) = \psi(x)e^{\frac{i}{\hbar}Et}\,, \quad -\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x)\,. \tag{3.5}$$

With the substitution (3.2), the stationary Schroedinger equation becomes

$$-i\frac{\hbar}{2m}S'' + \frac{1}{2m}S'^2 = E - V\,. \tag{3.6}$$

Let us write S as a formal series with respect to $\hbar$:

$$S = \sum_{n=0}^{\infty}\left(\frac{\hbar}{i}\right)^n S_n\,. \tag{3.7}$$

Plugging this back to Eq. (3.6) and extracting the contributions with different powers of $\hbar$, one obtains an infinite chain of equations for S_n, $n = 0,1,2,....$ These equations can be solved iteratively, since any of them contains terms in the expansion (10.18) only up to the corresponding order in $\hbar$. To the order $\hbar^0$, we have

$$\frac{1}{2m}\left(S_0'\right)^2 = E - V\,. \tag{3.8}$$

The solution to this equation is

$$S_0 = \pm\int dx\, p(x)\,, \quad p(x) = \sqrt{2m(E-V(x))}\,. \tag{3.9}$$

In classical mechanics, p is a momentum of the particle moving in the potential $V(x)$. Then, S_0 is just a coordinate part of the action of the particle. Restoring time-dependence, one obtains the full action

$$S_0(x,t) = \int (dx\, p - dt\, E)\,. \tag{3.10}$$

Note that the classical interpretation requires for p to be real, hence restricting the particle to move in the region $E > V(x)$.

Extracting the first order in $\hbar$ gives

$$-i\frac{\hbar}{2m}S_0'' + \frac{\hbar}{i}\frac{1}{2m}2S_0'S_1' = 0 \quad \Rightarrow \quad S_1' = -\frac{S_0''}{2S_0'}\,. \tag{3.11}$$

The last expression can be integrated explicitly, yielding

$$S_1 = -\frac{1}{2}\log S_0' + \text{const} = \log\frac{1}{\sqrt{p}} + \text{const}\,. \tag{3.12}$$

Combining S_0 and S_1, one obtains the leading-order expression for the semiclassical wavefunction,

$$\psi(x) = \frac{C_1}{\sqrt{p(x)}}\exp\left(\frac{i}{\hbar}\int p(x)dx\right) + \frac{C_2}{\sqrt{p(x)}}\exp\left(-\frac{i}{\hbar}\int p(x)dx\right)\,. \tag{3.13}$$

It is also known as the physical optics approximation. Note that to obtain the leading-order wavefunction, one should go to the order $\hbar^1$ in the series (10.18), since, after multiplying by $i/\hbar$ in Eq. (3.2), the term S_1 has no factor suppressing it.

3.2 Validity of the semiclassical approximation

It is not easy to prove that truncating the series (10.18) after a finite amount of terms gives a good and controllable approximation to the wavefunction (3.2). One reason for this is that in the limit $\hbar = 0$ Eq. (3.6) changes the order. In this sense, the perturbation theory with respect to $\hbar$ is singular. One can also see this from Eq. (3.2): unless $S_0 = 0$, at $\hbar = 0$ the function ψ ceases to exist. Nevertheless, asymptotic analysis and numerical calculations show that the WKB method works very well on practice. Then, for the truncation of the series (10.18) to be accurate, one should require the dropped terms to be small compared to the kept terms uniformly in x, that is

$$\begin{aligned} S_1(x) &\ll \frac{1}{\hbar}S_0(x)\,,\\ \hbar S_2(x) &\ll S_1(x)\,,\\ &\ldots\\ \hbar^n S_{n+1}(x) &\ll \hbar^{n-1}S_n(x)\,,\\ &\ldots \end{aligned} \tag{3.14}$$

These conditions are necessary but not *sufficient* for the semiclassical approximation to hold. Indeed, since the series (3.2) appears in the exponent of ψ, one should also require

$$\hbar^i S_{i+1}(x) \ll 1\,, \quad \text{for all } \; i > k \tag{3.15}$$

for the k'th order approximation to be legitimate.

In the exercises, we explore some of the conditions above and discuss the accuracy of the leading-order WKB approximation in detail. Here, let us derive one validity condition which follows from a different perspective but which has a clear physical meaning. To this end, notice that in Eq. (3.11) the $\hbar^1$-term can be neglected provided that

$$\left|\hbar S_0''\right| \ll \left|S_0'^2\right|\,. \tag{3.16}$$

In view of Eq. (3.9) this implies

$$\left|\frac{d}{dx}\left(\frac{\hbar}{p(x)}\right)\right| \ll 1\,. \tag{3.17}$$

In the last expression we recognize the de Broglie wavelength of the particle,

$$\lambda(x) = \frac{2\pi\hbar}{p(x)}\,. \tag{3.18}$$

Hence, Eq. (3.17) can be written as

$$|\lambda'(x)| \ll 1 \,. \tag{3.19}$$

This condition means that the relative change of the de Broglie wavelength over the distance of this wavelength must be small. Since the wavelength is determined by the momentum,

$$\lambda = \frac{\hbar}{p} \,, \tag{3.20}$$

and the change of the momentum is determined by the change of the potential, the inequality (3.19), in fact, means that the potential $V(x)$ must be smooth enough, so that its variation at one wavelength of the particle can be neglected. However, regardless the smoothness of the potential, the condition (3.19) is inevitably violated in the regions where the momentum p tends to zero. According to Eq. (3.9), this happens near the points where $E = V(x)$. These are so-called turning points, and we proceed to their study below.

3.3 Turning points

Let us look again at the semiclassical wavefunction (3.13). If $p(x)$ is treated as a classical momentum, the only regions where the particle can propagate are those for which $E > V(x)$. In quantum physics, however, the wavefunction can be non-zero in classically forbidden regions, i.e. when $E < V(x)$. To see how the semiclassical wavefunction looks like in the classically allowed and classically forbidden regions, consider a one-well potential shown in figure 3.1. Let the particle be confined in the well of the potential. The classically allowed region is defined by

$$E > V(x) \,, \;\; p^2(x) > 0 \;\; \Rightarrow \;\; x_1 < x < x_2 \,. \tag{3.21}$$

In this region, the wavefunction (3.13) shows an oscillating behavior,

$$\psi_{CA} = \frac{C_1}{\sqrt{p}} \exp\left(\frac{i}{\hbar}\int p dx\right) + \frac{C_2}{\sqrt{p}} \exp\left(-\frac{i}{\hbar}\int p dx\right) \,, \tag{3.22}$$

where C_1 and C_2 are constants determined from the boundary conditions to be discussed later. The probability to find the particle at the position x within the classically allowed region behaves as $|\psi_{CA}(x)|^2 \propto 1/p(x)$. This has a clear physical interpretation: the time the particle spends in a small spatial segment $(x, x+dx)$ is inversely proportional to its momentum or, equivalently, to its velocity $v(x) = p(x)/m$, as is expected from classical mechanics.

The regions of x for which

$$E < V(x) \,, \;\; p^2(x) < 0 \;\; \Rightarrow \;\; x < x_1 \text{ and } x > x_2 \tag{3.23}$$

are forbidden for classical motion. In these regions, the semiclassical wavefunction is still given by Eq. (3.13), but, given that the momentum is now purely imaginary, it can be rewritten as

$$\psi_{CF} = \frac{C_1'}{\sqrt{|p|}} \exp\left(-\frac{1}{\hbar}\int |p| dx\right) + \frac{C_2'}{\sqrt{|p|}} \exp\left(\frac{1}{\hbar}\int |p| dx\right) \,. \tag{3.24}$$

Again, the constants C_1' and C_2' are found by imposing appropriate boundary conditions. The latter must be chosen so that $|\psi_{CF}(x)|$ decays exponentially fast at $x < x_1$ or $x > x_2$. This comes from the requirement for the wavefunction of the particle bound in the potential to be normalizable and from our intuition that the probability $|\psi_{CF}(x)|$ to find the particle outside the classically allowed region must be suppressed.

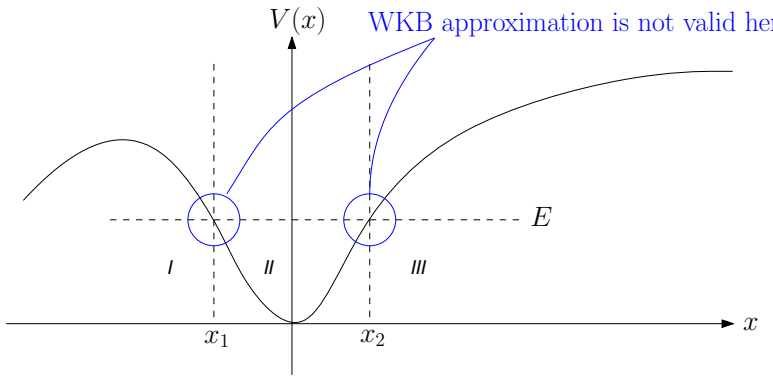


Figure 3.1: Classically allowed and classically forbidden regions of the potential $V(x)$.

From figure 3.1 we see that the points x_1 and x_2 are limiting points of the motion of the classical particle. At them, $v(x_{1,2}) = 0$, and the particle changes the direction of motion. For this reason, they are called turning points. Since near the turning points the momentum goes to zero, the semiclassical description breaks down and the expression (3.13) is not valid any more. If we want to build the wavefunction on the entire x-axis, we must learn how to match its different pieces, represented by Eq. (3.13), across the turning points. One way to proceed is to notice that near x_1 or x_2 the potential can be approximated by a linear function,

$$V(x) = E + F(x - x_{1,2}) + \mathcal{O}((x - x_{1,2})^2) \,, \quad F = \left.\frac{dV}{dx}\right|_{x=x_{1,2}} \,, \tag{3.25}$$

and the Schroedinger equation can be approximated as

$$-\frac{\hbar^2}{2m}\psi'' + F(x - x_{1,2})\psi = 0 \quad \text{close to} \quad x = x_{1,2} \,. \tag{3.26}$$

The latter equation admits an exact solution. This solution must be matched smoothly with the semiclassical wavefunction (3.13) to the both sides from the turning point. The matching and normalization conditions and the requirement of an exponential fall-off in the classically forbidden regions determine uniquely the constants in Eqs. (3.22), (3.24), thus selecting a unique semiclassical solution. In addendum A we use the outlined approach to solve the one-turning point problem. In the next lecture we will follow another route of bypassing the turning points.

Addendum A Here we consider the one-turning point problem to demonstrate how one can match the semiclassical wavefunctions in the two regions by using an exact solution of the Schroedinger equation at the turning point which we conveniently set to $x = 0$. Let us also put $m = 1$. We assume that the first derivative of the potential does not vanish at the turning point:

$$E - V(x) = Fx + Gx^2 + \mathcal{O}(x^3) \,. \tag{3.27}$$

Choose $F > 0$, so that $x > 0$ is the classically forbidden region, and $x < 0$ is the classically allowed region.

At $x > 0$, the semiclassical wavefuntion takes the form

$$\psi_{CF} = \frac{C}{\sqrt{|p|}} e^{-\frac{1}{\hbar}\int_0^x dx\, p} . \tag{3.28}$$

To compare it with the exact solution of the Schroedinger equation with the linearised potential, one must find the region where, on the one hand, the leading-order semiclassical approximation is valid and, on the other hand, the linear approximation of the potential is applicable. Let us start with the second condition. With the potential (3.27), the momentum becomes

$$|p| = 2F^{1/2}x^{1/2} + GF^{-1/2}x^{3/2} + \mathcal{O}(x^{5/2}) . \tag{3.29}$$

To the leading order in x, the wavefunction (3.28) is

$$\psi_{CF} = C2^{-1/2}F^{-1/4}x^{-1/4}e^{-\frac{1}{\hbar}\frac{2^{3/2}}{3}F^{1/2}x^{3/2}} . \tag{3.30}$$

We require the correction to Eq. (3.30) coming from the quadratic part of the potential to be small. This implies

$$x \ll 2FG^{-1} , \quad x \ll \hbar^{2/5}G^{-2/5}F^{1/5} . \tag{3.31}$$

Next, within the region of x set by Eqs. (3.31), we find the subregion where the leading-order semiclassical approximation is valid. According to Eqs. (3.14), (3.15), one should require that

$$|S_1| \ll |S_0/\hbar| , \quad |\hbar S_2| \ll |S_1| , \quad |\hbar S_2| \ll 1 . \tag{3.32}$$

This yields the condition (see Exercise 1.1)

$$x \gg \hbar^{2/3}F^{-1/3} . \tag{3.33}$$

Overall, Eq. (3.30) is valid in the interval

$$\hbar^{2/3}F^{-1/3} \ll x \ll \hbar^{2/5}G^{-2/5}F^{1/5} . \tag{3.34}$$

Given F and G finite, this inequality can always be satisfied for sufficiently small $\hbar$.
Let us now turn to the region around the turning point. In the Schroedinger equation

$$-\frac{\hbar^2}{2}\psi'' = Fx\psi \tag{3.35}$$

make a change of variable

$$t = 2^{1/3}\hbar^{-2/3}F^{1/3}x \tag{3.36}$$

to obtain

$$\frac{d^2\psi}{dt^2} = t\psi . \tag{3.37}$$

The general solution of this equation is expressed through Airy functions [2],

$$\psi(t) = D\,\mathrm{Ai}(t) + E\,\mathrm{Bi}(t) . \tag{3.38}$$

So far nothing in this expression resembles Eq. (3.30). But let us consider the asymptotic behaviour of the Airy functions at large positive argument. The appropriate formulas are

$$\mathrm{Ai}(t) \sim \frac{1}{2\sqrt{\pi}}t^{-1/4}e^{-2t^{3/2}/3} , \quad \mathrm{Bi}(t) \sim \frac{1}{\sqrt{\pi}}t^{-1/4}e^{2t^{3/2}/3} , \quad t \to \infty . \tag{3.39}$$

The solution (3.38) becomes, in terms of x,

$$\psi(x) = \frac{1}{\sqrt{\pi}}2^{-1/12}\hbar^{1/6}F^{-1/12}x^{-1/4}\left(\frac{1}{2}D\,e^{-2^{3/2}\hbar^{-1}F^{1/2}x^{3/2}/3} + E\,e^{2^{3/2}\hbar^{-1}F^{1/2}x^{3/2}/3}\right) . \tag{3.40}$$

This is valid provided that, first, the potential is well approximated by the linear function, $x \ll 2FG^{-1}$, and, second, the argument of the Airy functions is large, that is

$$\hbar^{-2/3}F^{1/3}x \gg 1 \;\;\Rightarrow\;\; x \gg \hbar^{2/3}F^{-1/3}\,. \tag{3.41}$$

We observe that the expressions (3.30) and (3.40) have a common region of validity defined by Eq. (3.34). Furthermore, their functional form is identical and they can, therefore, be matched. Namely,

$$D = C\cdot\pi^{/2}2^{7/12}F^{-1/6}\hbar^{-1/6}\,,\quad E=0\,. \tag{3.42}$$

We now repeat the above steps to match the solution (3.38) with the semiclassical wavefunction ψ_{CA} in the classically allowed region:

$$\psi_{CA} = \frac{C_1}{\sqrt{p}}e^{\frac{i}{\hbar}\int_x^0 dx\,p} + \frac{C_2}{\sqrt{p}}e^{-\frac{i}{\hbar}\int_x^0 dx\,p}\,. \tag{3.43}$$

In the region $\hbar^{2/3}F^{-1/3} \ll |x| \ll \hbar^{2/5}G^{-2/5}F^{1/5}$, the semiclassical wave function takes the form

$$\psi_{CA} = (2F|x|)^{-1/4}\left(C_1e^{-\frac{i}{\hbar}\frac{2^{3/2}}{3}F^{1/2}|x|^{3/2}} + C_2e^{\frac{i}{\hbar}\frac{2^{3/2}}{3}F^{1/2}|x|^{3/2}}\right)\,. \tag{3.44}$$

On the other hand, the asymptotics of the Airy functions at large negative argument are

$$\mathrm{Ai}(t) = \frac{1}{\sqrt{\pi}}|t|^{-1/4}\sin\left(\frac{2}{3}|t|^{3/2}+\frac{\pi}{4}\right)\,,\quad \mathrm{Bi}(t) = \frac{1}{\sqrt{\pi}}|t|^{-1/4}\cos\left(\frac{2}{3}|t|^{3/2}+\frac{\pi}{4}\right)\,,\;\; t\to-\infty\,. \tag{3.45}$$

Matching Eqs. (3.44) and (3.45), we obtain

$$C_1 = \hbar^{1/6}F^{1/6}2^{-7/12}\pi^{-1/2}e^{-\frac{i\pi}{4}}(E+iD)\,,\quad C_2 = \hbar^{1/6}F^{1/6}2^{-7/12}\pi^{-1/2}e^{\frac{i\pi}{4}}(E-iD)\,. \tag{3.46}$$

Finally, using Eqs. (3.42), we express the coefficients C_1, C_2 in Eq. (4.11) with the coefficient C in Eq. (3.28),

$$C_1 = Ce^{\frac{i\pi}{4}}\,,\quad C_1 = Ce^{-\frac{i\pi}{4}}\,, \tag{3.47}$$

hence,

$$\psi_{CA} = \frac{2C}{\sqrt{p}}\cos\left(\frac{i}{\hbar}\int_x^0 dx\,p + \frac{\pi}{4}\right)\,. \tag{3.48}$$

The only unknown parameter here is the constant C which is found from the normalization condition.

▪ **Exercise 3.1 — On validity of the leading-order (LO) WKB approximation.** Consider the semiclassical expansion of the wave function

$$\psi = e^{\frac{i}{\hbar}S}\,,\quad S = S_0 + \frac{\hbar}{i}S_1 + \left(\frac{\hbar}{i}\right)^2 S_2 + \ldots\,. \tag{3.49}$$

It was shown that one necessary applicability condition of the LO semiclassical approximation

$$\psi \approx e^{\frac{i}{\hbar}(S_0+\frac{\hbar}{i}S_1)} \tag{3.50}$$

is written as $|\lambda'| \ll 1$, where $\lambda = \hbar/p$ is the de Broglie wave length. In this exercise, we have a look at one more condition, $|\hbar S_2| \ll 1$.

1. Expanding the Schrödinger equation for ψ up to the second order in $\hbar$, find S_2' in terms of S_0' and S_1'. Rewrite it through the momentum p and its derivatives; through the energy of the particle E, the potential V and its derivatives.
2. Show that the condition $|\hbar S_2| \ll 1$ follows from $|\lambda'| \ll 1$ and $\int^x |\lambda'^2 \lambda^{-1}|\, dx \ll 1$.
3. From the condition $|\lambda'| \ll 1$ obtain the following inequality,

$$\left| \frac{\delta A}{T_{kin}} \right| \ll 1 \,, \tag{3.51}$$

where δA is the work done by a force $F = -V'$ over a distance λ, and T_{kin} is the kinetic energy of the particle.

▪

▪ **Exercise 3.2 — On accuracy of the LO WKB approximation.** Consider a particle of unit mass and energy V_0, moving in the potential

$$V(x) = \begin{cases} 0 \,, & x < 0 \,, \\ V_0 \sqrt{\dfrac{x}{x_0}} \,, & x > 0 \,. \end{cases} \tag{3.52}$$

1. Find the LO WKB wave function of the particle in the region $x > x_0$.
2. Find how small or large one should take V_0 to be sure that the LO approximation of the wave function is accurate to 1 percent for all $x > 2x_0$.

▪

▪ **Exercise 3.3 — On the asymptote of the potential in WKB approximation.** Consider a particle of zero energy, moving in a potential $V(x)$ shown schematically in Fig. 3.2. Assume that $V(x)$ approaches a constant negative value at $x \to -\infty$, and that its behavior at large positive x is of the form

$$V(x) \sim x^{-n} \,, \quad n > 0 \,, \quad x \to \infty \,. \tag{3.53}$$

1. Give a constraint on possible values of n, that ensures the validity of the LO WKB approximation of the decaying wave function in the limit $x \to \infty$.

Suppose now that the asymptotics of the potential at large positive x is

$$V(x) \sim \left(\frac{\log x}{x} \right)^2 \,. \tag{3.54}$$

2. Is it legitimate to use WKB theory to predict the large-x behavior of the decaying wave function?

▪

▪ **Exercise 3.4 — Numerical check of the LO WKB.** Consider the particle of unit mass and zero energy in the potential (all quantities below are assumed to be properly normalized)

$$V(x) \sim \sinh x \, (\cosh x)^2 \,. \tag{3.55}$$

Assume the following boundary conditions for the wavefunction: $\psi(+\infty) = 0$, $\psi(0) = 1$.

1. Construct the LO WKB wavefunction of the particle in the classically allowed and classically forbidden regions.
2. Solve the Schroedinger equation with the potential (3.55) numerically and check the agreement with the WKB solution at different values of $\hbar$.

▪

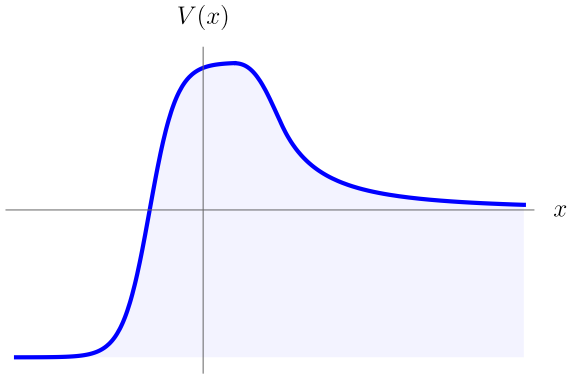


Figure 3.2: The potential

▪ **Exercise 3.5 — WKB expansion beyond the LO.** The physical optics approximation of the amplitude (3.13) can be corrected by successive calculation of higher-order terms in the expansion (10.18). These terms exhibit some interesting properties which, as we will see later, are important when computing energy levels of a particle in a potential.

1. Obtain an iterative expression for S'_n through $S'_0, \ldots, S'_{n-1}$.
2. Show that all *odd* terms S'_{2k+1} are
   (a) real (and, hence, do not contribute to the phase of the wavefunction),
   (b) total derivatives.

▪

▪ **Exercise 3.6 — One way of matching the semiclassical wavefunctions.** Fill the gaps in the exposition in Addendum A: derive Eqs. (3.30), (3.31), (3.33), (3.44), (3.46) and (4.10). ▪

Lecture 4

> Matching condition of the semiclassical wavefunctions and its applicability; normalization of the semiclassical wavefunction; Bohr-Sommerfeld quantization condition.

4.1 Matching the semiclassical wavefunctions across the turning points

By the end of lecture 5, we were left with the question of how to match the semiclassical wavefunction in the classically forbidden region with that in the classically allowed region. The problem is that near the turning points the WKB approximation breaks down. In what follows, we will assume that it is nevertheless valid close enough to the turning points, in the regions where the potential can be approximated by a linear function, see section 4.2 for the quantitative condition. Let us consider first the one-turning point problem at $x = x_0$, so that

$$V(x) = E + \left.\frac{dV}{dx}\right|_{x_0} (x - x_0) + \mathcal{O}((x-x_0)^2) \approx E + F(x-x_0) \,. \tag{4.1}$$

Let $F > 0$, then

$$\psi_{CA} = \frac{C_1}{\sqrt{p}} e^{-\frac{i}{\hbar}\int_x^{x_0} dx'\, p} + \frac{C_2}{\sqrt{p}} e^{\frac{i}{\hbar}\int_x^{x_0} dx'\, p} \,, \tag{4.2}$$

$$\psi_{CF} = \frac{C}{2\sqrt{|p|}} e^{-\frac{1}{\hbar}\int_{x_0}^{x} dx'\, |p|} \,, \tag{4.3}$$

where C, $C_{1,2}$ are real constants. In writing Eq. (4.3), we imposed the boundary condition

$$\psi_{CF}(+\infty) = 0 \,, \tag{4.4}$$

which is necessary for the wavefunction to be normalizable. On the other hand, in Eq. (4.2) no boundary conditions are imposed. Since ψ_{CA} and ψ_{CF} approximate the same solution of the exact Schroedinger equation, the requirement (4.4) must be transferred somehow to the condition on the constants $C_{1,2}$. That is, $C_{1,2}$ must be expressed through C. Our goal is to find these expressions. Note here the directional character of the matching procedure: it is important to start with the wavefunction in the classically forbidden region ψ_{CF}, since there is an *exact* boundary condition imposed on it.

To do the matching, notice that, although one cannot continue the function ψ_{CF} to the interval $x < x_0$ straight through the singular point, one can do so if the singularity is bypassed. To bypass

the point $x = x_0$, we extend the domain of ψ_{CF} from the interval $x_0 < x < \infty$ to the complex plane and continue the function analytically to that plane:

$$x = \mathrm{Re}\, z\,, \quad \psi_{CF}(x) \Rightarrow \tilde{\psi}_{CF}(z) \text{ such that } \tilde{\psi}_{CF}(z) = \psi_{CF}(x) \text{ for } \mathrm{Re}\, z = x\,,\ \mathrm{Im}\, z = 0\,,\ x_0 < x < \infty\,. \tag{4.5}$$

The continued function $\tilde{\psi}_{CF}$ is defined everywhere except $z = x_0$ and, in particular, it is defined at the points $\mathrm{Re}\, z < x_0$, $\mathrm{Im}\, z = 0$, where it should be matched with Eq. (4.2). This is the idea of the matching procedure we are going to implement.

Let us pause here and make an important observation. The solution of the *exact* Schroedinger equation does not suffer from singularity at the turning point. The singularity is an artefact of truncating the series (10.18) after a finite amount of terms. Hence, the exact wavefunction is analytic in the entire complex plane, and its continuation to that plane from any interval on the real axis is unambiguous. The semiclassical wavefunction $\tilde{\psi}_{CF}$, on the other hand, is not analytic in the complex plane, since it has the irremovable singularity at the turning point. Hence, its values in the classically allowed region $x < x_0$ *will* depend on the way we continue it from the classically forbidden region $x > x_0$. Different answers will correspond to different particular solutions, and an appropriate linear combination of them will give the semiclassical wavefunction at $x < x_0$.

We now compute $\tilde{\psi}_{CF}$ at $x < x_0$ given that ψ_{CF} takes the form (4.3). In the region of z where the linear approximation for the potential works, $\tilde{\psi}_{CF}$ is written as

$$\tilde{\psi}_{CF}(z) = \frac{C}{2}(2mF)^{-1/4} z^{-1/4} e^{-\frac{2}{3\hbar}(2mF)^{1/2} z^{3/2}}\,. \tag{4.6}$$

At the points $\mathrm{Re}\, z > x_0$, $\mathrm{Im}\, z = 0$, this reduces to Eq. (4.3). To see what values the function (4.6) takes at $\mathrm{Re}\, z < x_0$, $\mathrm{Im}\, z = 0$, we write

$$z = \rho e^{i\phi}\,. \tag{4.7}$$

Let $\rho = \mathrm{const}$. Then, at $\phi = 0$ the point z belongs to the interval $\mathrm{Re}\, z > x_0$, $\mathrm{Im}\, z = 0$, and at $\phi = \pm\pi$ it belongs to the interval $\mathrm{Re}\, z < x_0$, $\mathrm{Im}\, z = 0$. Hence, one should substitute $z = \rho e^{\pm i\pi}$ into Eq. (4.6). Choosing "+" sign corresponds to bypassing the turning point counter-clockwise, and choosing "-" sign corresponds to bypassing it clockwise (see figure 4.1). We obtain

$$\begin{aligned} \tilde{\psi}_{CF}(\rho e^{i\pi}) &= \frac{C}{2(2mF)^{1/4}} \frac{1}{\rho^{1/4} e^{i\pi/4}} \exp\left[-\frac{2}{3\hbar}(2mF)^{1/2}\rho^{3/2} e^{3i\pi/2}\right] \\ &= \frac{C}{2\sqrt{p}} \exp\left[+\frac{i}{\hbar}\int_x^{x_0} p\,dx + \frac{i\pi}{4}\right]\,, \end{aligned} \tag{4.8}$$

and

$$\begin{aligned} \tilde{\psi}_{CF}(\rho e^{-i\pi}) &= \frac{C}{2(2mF)^{1/4}} \frac{1}{\rho^{1/4} e^{-i\pi/4}} \exp\left[-\frac{2}{3\hbar}(2mF)^{1/2}\rho^{3/2} e^{-3i\pi/2}\right] \\ &= \frac{C}{2\sqrt{p}} \exp\left[-\frac{i}{\hbar}\int_x^{x_0} p\,dx + \frac{i\pi}{4}\right]\,. \end{aligned} \tag{4.9}$$

Comparing these expressions with Eq. (4.2), we see that one should choose

$$C_1 = \frac{C}{2} e^{i\pi/4}\,, \quad C_2 = \frac{C}{2} e^{-i\pi/4}\,. \tag{4.10}$$

The wavefunction ψ_{CA} can then be written as

$$\psi_{CA} = \frac{C}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_x^{x_0} p\,dx - \frac{\pi}{4}\right)\,. \tag{4.11}$$

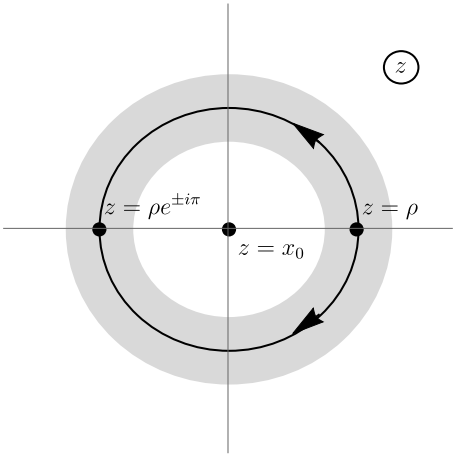


Figure 4.1: Two continuation contours from the classically forbidden to the classically allowed regions. The gray ring denotes the region where both the semiclassical approximation and the linear approximation for the potential work.

Eqs. (4.3) and (4.11) determine the semiclassical wavefunction up to the normalization constant C at all x except the proximity of the turning point. In addendum A it is explained in more detail why the C_1-term in Eq. (4.2) is restored by continuing clockwise from the classically forbidden region, and the C_2-term — by continuing counter-clockwise.

4.2 Applicability of the matching procedure

Let us discuss the assumption we made when approximating the potential $V(x)$ by a linear function in Eq. (4.1). This approximation works if the second derivative term is small compared to the linear term:

$$\left|\frac{1}{2}V''(x_0)(x-x_0)^2\right| \ll \left|V'(x_0)(x-x_0)\right| \;\;\Rightarrow\;\; |x-x_0| \ll \left|\frac{2V'(x_0)}{V''(x_0)}\right| . \tag{4.12}$$

In the region where Eq. (4.12) is satisfied, the applicability condition (3.19) of the leading-order semiclassical approximation reduces to

$$\left|\frac{\hbar}{\sqrt{2m|V'(x_0)|}}\frac{1}{2}\frac{1}{(x-x_0)^{3/2}}\right| \ll 1 . \tag{4.13}$$

The conditions (4.12) and (4.13) can be satisfied simultaneously for some $|x-x_0|$ if (we omit the order one coefficients)

$$|V'(x_0)|^2 \gg \frac{\hbar}{\sqrt{m}}|V''(x_0)|^{3/2} . \tag{4.14}$$

Two comments are in order. First, it is easy to provide an example of the potential for which the condition (4.14) is not satisfied. The potential in figure 4.2(1) violates it because the first non-zero term in the Taylor expansion of $E-V(x)$ around x_0 is of the third order in $x-x_0$. The result of analytic continuation of the function (4.6) around the turning point depends on the powers of $|z|$ it contains, and those powers are determined by the form of the potential near x_0. Hence, Eq. (4.11) is not valid in this case, but the method we used remains in force, and the procedure can be repeated with the new form of the function (4.6), see exercise 4.6. Second, consider the potential depicted in figure 4.2(2). In the limit $V(x) = \infty$ for $x > x_0$, the wavefunction in the classically forbidden region

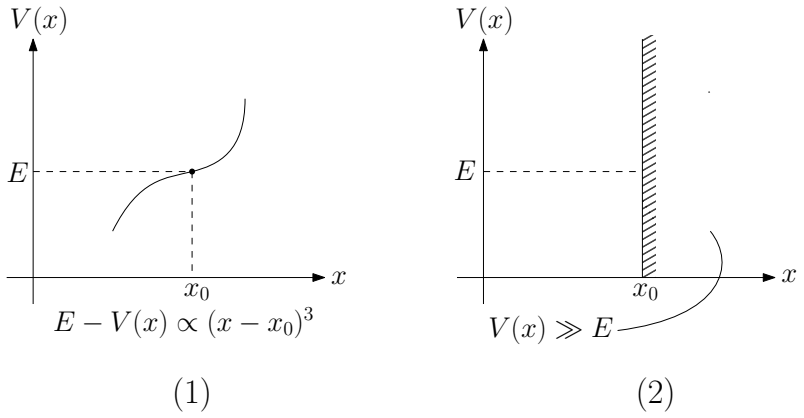


Figure 4.2: Examples of the potentials for which the matching procedure described in section 4.1 does not work.

ψ_{CF} must be zero. An attempt to continue ψ_{CF} to the classically allowed region then fails, since ψ_{CA} is clearly non-zero, contrary to what follows from Eqs. (4.10). The failure happens because the area where the polynomial approximation of the potential and the semiclassical approximation hold together does not contain the path leading from one region to another. Instead, one should take the boundary condition $\psi_{CA}(x_0) = 0$, which leads to (see also exercise 4.3)

$$\psi_{CA} \propto \cos\left(\frac{1}{\hbar}\int_x^{x_0} |p|dx - \frac{\pi}{2}\right) . \tag{4.15}$$

Note finally, that, in general, the semiclassical wavefunction in the classically allowed region (4.2) can be written as

$$\psi_{CA} \propto \cos\left(\frac{1}{\hbar}\int_x^{x_0} dx\,|p| - \varphi\right) . \tag{4.16}$$

The coefficient in front of the cos is found from the normalization condition, whereas the phase φ is determined by the structure of the turning point.

4.3 Normalization of the semiclassical wavefunction

To find the coefficient C in Eqs. (4.3) and (4.11), one should impose an additional condition on the semiclassical wavefunction. Here we consider the case when the particle is confined in the well of the potential, as is shown in figure 3.1, hence both at $x \to +\infty$ and $x \to -\infty$ its wavefunction must go to zero. In the classically allowed region $x_1 < x < x_2$ we can write

$$\psi_{\rm CA} = \frac{C}{\sqrt{|p|}} \cos\left(\frac{1}{\hbar}\int_{x_1}^{x} |p|dx - \varphi\right) . \tag{4.17}$$

Then, neglecting the exponential tails in the classically forbidden regions $x < x_1$, $x > x_2$, from the normalization condition we have

$$\begin{aligned} 1 \approx \int |\psi_{\rm CA}|^2 dx &= \int_{x_1}^{x_2} dx \frac{C^2}{p} \cos^2\left(\frac{1}{\hbar}\int_{x_1}^{x} |p|dx - \phi\right) \\ &\approx \frac{1}{2}C^2 \int_{x_1}^{x_2} \frac{dx}{|p|} = \frac{1}{2}C^2 \int_{x_1}^{x_2} \frac{dx}{m dx/dt} = \frac{1}{2}C^2 \frac{1}{m}\frac{T}{2} . \end{aligned} \tag{4.18}$$

In going from the first to second line, we used the fact that cos oscillates rapidly compared to the charactersitic scale at which the momentum p varies, as it should for the semiclassical

approximation to work. In the last expression, T is the classical period of oscillations of the particle in the potential well. Thus,

$$C = 2\sqrt{\frac{m}{T}}\,. \tag{4.19}$$

4.4 Bohr-Sommerfeld quantization condition

Consider again the potential shown in figure 3.1. In the classically forbidden regions I and III, the semiclassical wavefunction takes the form

$$\psi_I = \frac{C}{2\sqrt{|p|}}\exp\left[-\frac{1}{\hbar}\int_x^{x_1}|p|dx'\right]\,, \qquad x < x_1\,, \tag{4.20}$$

$$\psi_{III} = \frac{\tilde{C}}{2\sqrt{|p|}}\exp\left[-\frac{1}{\hbar}\int_{x_2}^{x}|p|dx'\right]\,, \qquad x_2 < x\,. \tag{4.21}$$

On the one hand, matching the solution in region III with that in the classically allowed region II gives

$$\psi_{II} = \frac{C}{\sqrt{p}}\cos\left[\frac{1}{\hbar}\int_x^{x_2}pdx' - \frac{\pi}{4}\right]\,, \qquad x_1 < x < x_2\,. \tag{4.22}$$

On the other hand, matching the solution in region I with that in region II leads to (see exercise 4.2)

$$\psi_{II} = \frac{\tilde{C}}{\sqrt{p}}\cos\left[\frac{1}{\hbar}\int_{x_1}^{x}pdx' - \frac{\pi}{4}\right]\,, \qquad x_1 < x < x_2\,. \tag{4.23}$$

The solution in region II should not, of course, depend on the way we obtain it. Therefore,

$$\cos\left[\frac{1}{\hbar}\int_x^{x_2}pdx' - \frac{\pi}{4}\right] = \pm\cos\left[\frac{1}{\hbar}\int_{x_1}^{x}pdx' - \frac{\pi}{4}\right]\,, \tag{4.24}$$

which implies

$$\frac{1}{\hbar}\int_{x_1}^{x}pdx' - \frac{\pi}{4} = \frac{1}{\hbar}\int_x^{x_2}pdx' - \frac{\pi}{4} + \pi n\,, \quad \text{or} \tag{4.25}$$

$$\frac{1}{\hbar}\int_{x_1}^{x}pdx' - \frac{\pi}{4} = -\left(\frac{1}{\hbar}\int_x^{x_2}pdx' - \frac{\pi}{4}\right) + \pi n\,. \tag{4.26}$$

The first of these equations cannot be satisfied at all x. The second leads to

$$\frac{1}{\hbar}\int_{x_1}^{x_2}pdx = \pi\left(n + \frac{1}{2}\right)\,. \tag{4.27}$$

This can be written as

$$\oint pdx = 2\pi\hbar\left(n + \frac{1}{2}\right)\,, \tag{4.28}$$

where the integration is performed over one period of classical oscillations. Eq. (4.28) is known as the Bohr-Sommerfeld quantization condition. Its applicability is determined by Eq. (4.14).

The Bohr-Sommerfeld quantization condition is a powerful tool that allows to compute semi-classical energy levels of a particle in a potential well. To demonstrate this, consider the harmonic oscillator,

$$V(x) = \frac{1}{2}m\omega^2 x^2 \,, \tag{4.29}$$

$$p(x) = \sqrt{2m\left(E - \frac{1}{2}m\omega^2 x^2\right)} \,. \tag{4.30}$$

The turning points are located at

$$\pm\left(\frac{2E}{m\omega^2}\right)^{1/2} \equiv \pm x_0 \,. \tag{4.31}$$

Applying the quantization condition gives

$$\begin{aligned} 2\pi\hbar\left(n+\frac{1}{2}\right) &= \oint p\,dx \\ &= 2\int_{-x_0}^{x_0} dx\,\sqrt{2m}\,\sqrt{E-\frac{1}{2}m\omega^2x^2} \\ &= 2\left(2m-\frac{1}{2}m\omega^2\right)^{1/2}\int_{-x_0}^{x_0} dx\left(x_0^2-x^2\right)^{1/2} \\ &= \frac{2\pi E}{\omega} \,. \end{aligned} \tag{4.32}$$

Thus,

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right) \,, \quad n = 0,1,2... \tag{4.33}$$

and we have reproduced the familiar formula for the energy levels of the harmonic oscillator. It is interesting to note that in this case the leading-order approximation gives the exact answer for all n, although the applicability condition (4.14) can only state that the approximation is accurate at large enough n, see exercise 4.4.

Addendum A

Let us see why changing the phase from 0 to $-\pi$ results in the C_1-term in Eq. (4.2), while changing from 0 to π leads to the C_2-term. Take the first term. In the linear approximation for the potential, its exponential part reads

$$\exp\left[-\frac{2i}{3\hbar}(2mF)^{1/2}\rho^{3/2}\left(\cos\frac{3\psi}{2}+i\sin\frac{3\psi}{2}\right)\right] \,. \tag{4.34}$$

Here the coordinates ρ and ψ are chosen so that the real point $x < x_0$ has $\psi = 0$. The real part of the expression under the exponent can be positive or negative depending on the value of ψ. Continuing Eq. (4.34) from $\psi = 0$ to $\psi = \pi$, we travel first through the region where the real part of the wavefunction is exponentially large,

$$\cos\frac{3\psi}{2} < 0 \;\text{ at }\; 0 < \psi < 2\pi/3 \,, \tag{4.35}$$

and then — through the region where it is exponentially small,

$$\cos\frac{3\psi}{2} > 0 \;\text{ at }\; 2\pi/3 < \psi < \pi \,. \tag{4.36}$$

Hence, this choice of the contour results in the exponentially small wavefunction in the classically forbidden region, which is consistent with the boundary condition at infinity, see the left panel of figure 4.3 for illustration. On the other hand, continuing the wavefunction from $\psi = 0$ to $\psi = -\pi$, we go through the region where the real part of Eq. (4.34) is exponentially small, followed by the region where it is exponentially large. As a result, we obtain the growing wavefunction in the classically forbidden region, which is inconsistent with the boundary condition at infinity. Thus, starting from Eq. (4.3), one should use the lower contour to arrive at the C_1-term in Eq. (4.2).

The reasoning can be repeated for the C_2-term. The only difference is the plus sign in the exponent in Eq. (4.34). Hence, the regions of large and small contributions are exchanged, and it is the upper contour (for which ψ changes from 0 to $-\pi$) which results in the exponentially small wavefunction in the classically forbidden region, see the right panel of figure 4.3 for illustration. Thus, by using the upper contour, one arrives from Eq. (4.3) to the C_2-term in Eq. (4.2).

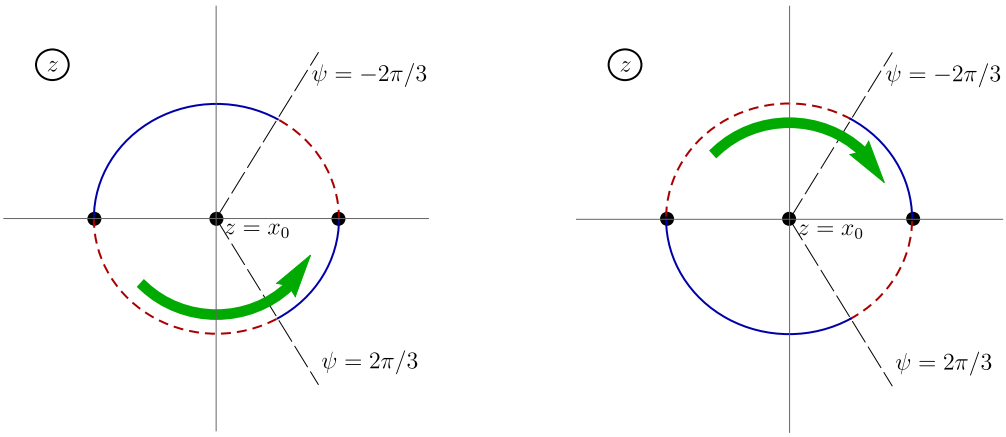


Figure 4.3: Left panel: behavior of the function (4.34) in the complex plane. Solid lines correspond to the regions where the function is exponentially small, dashed lines — to the regions where it is exponentially large. The arrow points the direction of continuation for which the wavefunction (4.3) in the classically forbidden region is reproduced. *Right panel:* the same for the function with the different sign in the exponent.

▪ **Exercise 4.1 — Quick dimensional analysis.** Check that both sides of Eq. (4.14) have the same dimension. ▪

▪ **Exercise 4.2 — The one-turning point problem.** In the classically forbidden region $x < x_0$, the LO WKB wave function is given by

$$\psi(x) = \frac{C}{2\sqrt{|p(x)|}} \exp\left(-\frac{1}{\hbar}\int_x^{x_0} |p(x')|dx'\right) . \tag{4.37}$$

1. Find the expression for this wave function in the classically allowed region $x > x_0$.

▪

▪ **Exercise 4.3 — Quantization rule in a half-space.** The Bohr-Sommerfeld quantization rule

$$\oint p dx = 2\pi\hbar\left(n + \frac{1}{2}\right) \tag{4.38}$$

was derived under the assumption that there are two turning points beyond which the classically forbidden regions lie and the wave function ψ falls off exponentially fast. This amounts to imposing

the boundary conditions $\psi(\pm\infty) = 0$ that are exact in any order in $\hbar$. What if a given physical problem requires other boundary data? For example, consider the following conditions,

$$\psi(\infty) = 0\,, \quad \psi(x) = 0\,, \;\; x \leqslant 0\,. \tag{4.39}$$

They imply that the potential in the problem is supplemented by an infinite wall at $x = 0$ beyond which no wave function can penetrate (see figure 4.4).

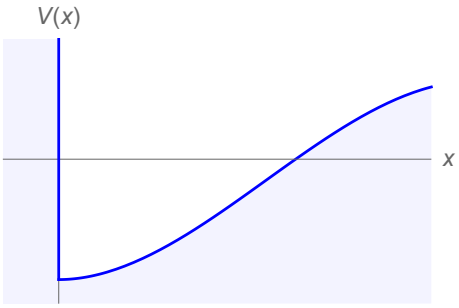


Figure 4.4: The infinite wall potential

1. Derive the quantization rule for bound states in this type of potentials.

The rule you have found has a natural application to computation of energy levels of three-dimensional systems possessing spherical symmetry. Indeed, the potential of the system in this case depends only on the radial coordinate r. If the potential is regular at $r = 0$, then for the wave functions with zero orbital momentum the problem reduces to solving the one-dimensional Schroedinger equation with $V = V(r)$ at $r > 0$, and $V = \infty$ at $r = 0$.

2. In the LO WKB approach, find energy levels of bottomonium — a pair of nonrelativistic quark and antiquark with masses $m_c = 4.98\,GeV$ placed in a linear potential $V = V_0 + kr$, with $V_0 = 5\,MeV$ and $k = 0.8\,GeV^2$.

▪

▪ **Exercise 4.4 — WKB spectrum of the Harmonic oscillator.** Consider a particle of mass m, moving in the potential $V(x) = \dfrac{1}{2} m\omega^2 x^2$.

1. Find for which values of E you can trust the result (4.33) according to the LO WKB applicability condition.

▪

▪ **Exercise 4.5 — WKB spectrum in power-like potential.** At large n, the qualitative dependence of the energy E_n of the n'th WKB bound state is of the form

$$E_n \sim n^\beta\,, \quad n \gg 1\,, \tag{4.40}$$

where the exponent β is determined by the potential. For example, from the previous exercise we know that for the harmonic oscillator $\beta = 1$. To analyze the range of possible values of β, consider the particle of mass m, confined in the potential

$$V(x) = V_0 \left| \frac{x}{x_0} \right|^\alpha\,, \quad \alpha > 0\,. \tag{4.41}$$

1. Find the LO WKB spectrum of the particle. Check that for $\alpha = 2$ the answer reduces to the spectrum of the harmonic oscillator.
   Hint: Use the formula

$$\int_0^1 \sqrt{1 - y^\alpha}\, dy = \frac{\sqrt{\pi}}{2} \frac{\Gamma(1 + \frac{1}{\alpha})}{\Gamma(\frac{3}{2} + \frac{1}{\alpha})}\,, \quad \alpha > 0\,, \tag{4.42}$$

where $\Gamma(z)$ is the Gamma function.

2. Plot the function $\beta = \beta(\alpha)$, where β is defined in eq. (4.40). What happens when $\alpha \to \infty$?

▪

▪ **Exercise 4.6 — The multifold one-turning point problem.** Consider the wave function continued from the classically forbidden region $x > 0$ to the classically allowed region $x < 0$ through the turning point of multiplicity $2k+1$, with k an integer number (see figure 4.5),

$$V(x) - E \sim x^{2k+1} \ , \quad |x| \ll 1 \ . \tag{4.43}$$

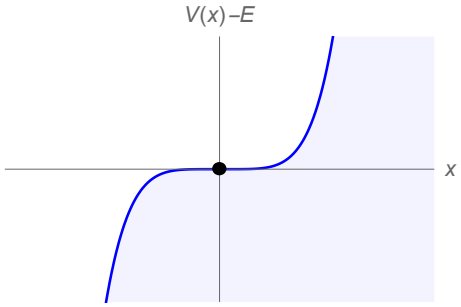


Figure 4.5: The turning point of high multiplicity

1. Find the LO WKB wave function of a particle at $x < 0$, if at $x > 0$ it is given by

$$\psi(x) = \frac{C}{2\sqrt{|p|}} \exp\left(-\frac{1}{\hbar}\left|\int_0^x p\,dx\right|\right) \ , \quad x > 0 \ . \tag{4.44}$$

▪

▪ **Exercise* 4.7 — Quantization rule beyond the LO.** Knowing the higher-order terms in the expansion of the semiclassical wave function enables us to improve the LO quantization rule (4.38). One can expect that the corrections to this rule are suppressed by the powers of $\hbar$, and that their successive calculation leads to the *exact* quantization rule of the form

$$\sum_{n=0}^{\infty} \hbar^n \delta_n = 2\pi\hbar\left(n + \frac{1}{2}\right) \ , \tag{4.45}$$

where each δ_n is some integral over the closed path enclosing the turning points x_1 and x_2. From Eq. (4.38) we see that

$$\delta_0 = \sqrt{2m} \oint \sqrt{E - V}\,dx \ . \tag{4.46}$$

Furthermore, we know that $\delta_{2k+1} = 0$ for any $k \geqslant 0$, since the corresponding terms in the expansion of the wave function are total derivatives and, hence, cannot contribute to the closed path integral. The challenge of this exercise is to compute the second-order term δ_2. To this end, we need to find the next-to-the-leading-order (NLO) WKB wave function ψ which is given by

$$\psi = e^{\frac{i}{\hbar}\left(S_0 + \frac{\hbar}{i}S_1 + \left(\frac{\hbar}{i}\right)^2 S_2\right)} \ . \tag{4.47}$$

To shorten the notations, denote by I and III the classically forbidden regions $x < x_1$ and $x > x_2$ accordingly, and by II — the classically allowed region $x_1 < x < x_2$.

1. Write the expressions for the NLO WKB wave functions ψ_1, ψ_2, and ψ_3 in the regions I, II, and III accordingly. Apply the boundary conditions $\psi_1(-\infty) = 0$, $\psi_3(\infty) = 0$.

2. Following the method explained in Addendum A of the previous lecture, continue the wavefunctions ψ_1 and ψ_3 to the classically allowed region. Equating the results, deduce the quantization rule. Write it in the form (4.45) and show that δ_2 can be reduced to

$$\delta_2 = -\frac{1}{24\sqrt{2m}}\frac{d}{dE}\oint \frac{V''}{\sqrt{E-V}}dx\,. \tag{4.48}$$

3. Compute δ_2 for the harmonic oscillator.

▪

Lecture 5

> the Planck formula; tunneling through a potential barrier; decay of a metastable state; splitting of energy levels in a double-well potential.

5.1 the Planck formula

The Bohr-Sommerfeld quantization rule states that the phase volume Γ occupied by a given stationary state in a potential well (the l.h.s. of Eq. (4.28)) contains an integer amount of elementary phase cells with $\Delta\Gamma = 2\pi\hbar$ (the r.h.s. of Eq. (4.28) up to the contribution from the ground state). Let us now compute the energy difference between two neighbouring stationary states. To this end, we differentiate Eq. (4.28) with respect to E:

$$\frac{\partial}{\partial E}\int_{x_1}^{x_2} p dx = p(x_2)\frac{\partial x_2}{\partial E} - p(x_1)\frac{\partial x_1}{\partial E} + \int_{x_1}^{x_2}\frac{\partial p}{\partial E}dx\,. \tag{5.1}$$

Since x_1 and x_2 are the turning points, $p(x_{1,2}) = 0$, and we are left with

$$\begin{aligned}\frac{\partial}{\partial E}\int_{x_1}^{x_2} p\,dx &= \int_{x_1}^{x_2}\frac{\partial}{\partial E}\sqrt{2m(E-V)}\,dx \\ &= \int_{x_1}^{x_2}\sqrt{\frac{m}{2(E-V)}}\,dx\,.\end{aligned} \tag{5.2}$$

In the last integral, we replace dx by dt using the definition of momentum

$$m\frac{dx}{dt} = \sqrt{2m(E-V)} \;\;\Rightarrow\;\; dx = dt\sqrt{\frac{2(E-V)}{m}}\,. \tag{5.3}$$

Hence,

$$\frac{\partial}{\partial E}\int_{x_1}^{x_2} p dx = \int_{t(x_1)}^{t(x_2)} dt = \frac{T}{2}\,, \tag{5.4}$$

where T is the classical period of oscillations of a particle in the well. Therefore,

$$\frac{\partial}{\partial E}\oint p dx = T\,. \tag{5.5}$$

Applying the Bohr-Sommerfeld quantization rule (4.28), we obtain

$$2\pi\hbar\frac{\partial n}{\partial E} = T \;\;\Rightarrow\;\; \Delta E = \hbar\omega\cdot\Delta n\,, \tag{5.6}$$

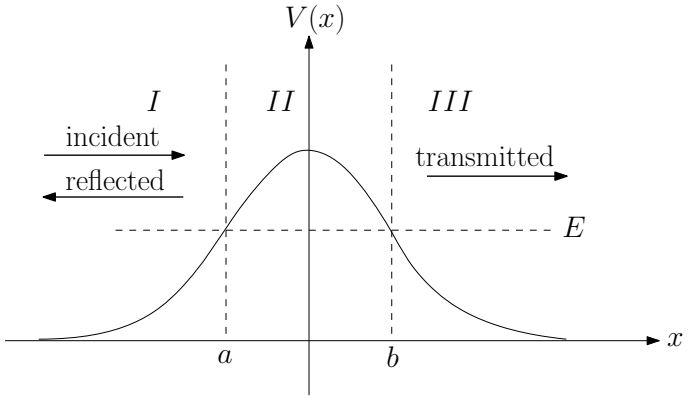


Figure 5.1: A particle coming from the left encounters a potential barrier $V(x)$.

where it was used that $\Delta E = \partial E/\partial n\, \Delta n|_{\Delta n=1}$. We conclude that the leading-order WKB approximation reproduces an exact result for the energy difference between the nearest energy levels — the Planck formula.

5.2 Tunneling through a potential barrier

Consider the one-dimensional potential shown in figure 5.1, with the asymptotics $V(x) \to 0$ at $x \to \pm\infty$. Let the incident steady flow of particles approach the central region of the potential — the barrier — from the left and scatter on it. Far from the barrier, the corresponding solution of the Schroedinger equation can be taken as a linear combination of plane waves:

$$\psi_{x\to-\infty} = e^{\frac{i}{\hbar}px} + Re^{-\frac{i}{\hbar}px}\,, \quad \psi_{x\to\infty} = De^{\frac{i}{\hbar}px}\,. \tag{5.7}$$

R and D are called the reflection and transmission coefficients respectively. If the energy of the particles is smaller than the height of the potential barrier, then the ratio of the transmitted to the incident probability fluxes determine the probability for the particle to tunnel through the barrier:

$$P = |D|^2\,. \tag{5.8}$$

Recall also that conservation of probability requires

$$|D|^2 + |R|^2 = 1\,. \tag{5.9}$$

Our goal in this section is to derive the reflection and transmission coefficients in the leading-order WKB approximation. Let a and b be the turning points separating regions I and III accessible for classical motion from region II in which tunneling occurs, see figure 5.1. We require no incoming wave in region III, which allows us to write

$$\psi_{III} = \frac{C}{\sqrt{p}} e^{\frac{i}{\hbar}\int_b^x dx'\, p}\,. \tag{5.10}$$

Let us continue this expression to region II. Approximating the potential by a linear function near the point $x = b$, we have

$$\int_b^x dx'\, p = \frac{2}{3}(-2mV'(b))^{1/2}(x-b)^{3/2}\,. \tag{5.11}$$

Proceeding as in the previous lecture, we extend the domain of ψ_{III} to the complex plane and denote $x-b=\rho e^{i\phi}$, so that $\phi=0$ corresponds to the point in the classically allowed region, and the point with $\phi=\pm\pi$ belongs to the classically forbidden region. Continuing counter-clockwise around $x=b$, one obtains

$$\begin{aligned}\tilde{\psi}_{III}(x)|_{x<b} &= e^{-\frac{i\pi}{4}}\frac{C}{\sqrt{|p|}}e^{\frac{1}{\hbar}\int_x^b dx'|p|} \\ &= e^{-\frac{i\pi}{4}}\frac{C}{\sqrt{|p|}}e^{\frac{1}{\hbar}\int_a^b dx|p|}e^{-\frac{1}{\hbar}\int_a^x dx'|p|}\,.\end{aligned} \tag{5.12}$$

Next, continuing in the clockwise direction leads to the contribution suppressed exponentially compared to the one just obtained. In the WKB approximation that contribution should be discarded, hence

$$\psi_{II}(x) = \tilde{\psi}_{III}(x)|_{x<b}\,. \tag{5.13}$$

The amplitude of the wavefunction (5.13) decays exponentially fast as x changes from the left to the right turning point. This is consistent with our expectation about the behaviour of particle's amplitude as the latter "propagates" under the barrier.

We now continue Eq. (5.13) to the classically allowed region I. This gives,

$$\begin{aligned}\psi_I(x) &= \frac{2C}{\sqrt{p}}e^{-\frac{i\pi}{4}}e^{\frac{1}{\hbar}\int_a^b dx|p|}\cos\left(\frac{1}{\hbar}\int_x^a dx\,p-\frac{\pi}{4}\right) \\ &= \frac{C}{\sqrt{p}}e^{\frac{1}{\hbar}\int_a^b dx|p|}\left(e^{\frac{i}{\hbar}\int_x^a dx\,p-\frac{i\pi}{4}}+e^{-\frac{i}{\hbar}\int_x^a dx\,p+\frac{i\pi}{4}}\right)\,.\end{aligned} \tag{5.14}$$

In this expression, the first term is identified with the incident wave, and the second term corresponds to the reflected wave. Far from the barrier, ψ_I and ψ_{III} can be written as

$$\psi_I = e^{\frac{i}{\hbar}\int_x^a dx\,p}+Re^{-\frac{i}{\hbar}\int_x^a dx\,p}\,,\quad \psi_{III}=De^{\frac{i}{\hbar}\int_b^x dx\,p}\,. \tag{5.15}$$

Comparing with Eqs. (5.10), (5.14), we find

$$R=e^{\frac{i\pi}{2}}\,,\quad D=e^{\frac{i\pi}{2}}e^{-\frac{1}{\hbar}\int_a^b dx\,|p|}\,. \tag{5.16}$$

As before, the probability for the particle to appear on the right side from the barrier is given by the ratio of the transmitted to the incident probability fluxes:

$$P=|D|^2=e^{-\frac{2}{\hbar}\int_a^b dx\,|p|}\,. \tag{5.17}$$

In deriving Eq. (5.17), it was important to assume that the integral in the exponent is large,

$$\frac{1}{\hbar}\int_a^b dx\,|p|\gg 1\,, \tag{5.18}$$

as otherwise the leading-order WKB looses its predictive power. This can also be understood by noticing that when the condition (5.18) is violated, the tunneling becomes unsuppressed, and higher-order corrections to the exponential in Eq. (5.17) cannot be neglected (see exercise 5.7). Eq. (5.18) implies, in particular, that

$$\frac{b-a}{\lambda}\gg 1\,, \tag{5.19}$$

i.e., roughly speaking, the width of the potential must exceed significantly the wavelength of the particle. Note finally that from Eq. (5.16) it follows that $|R|^2=1$. This does not contradict

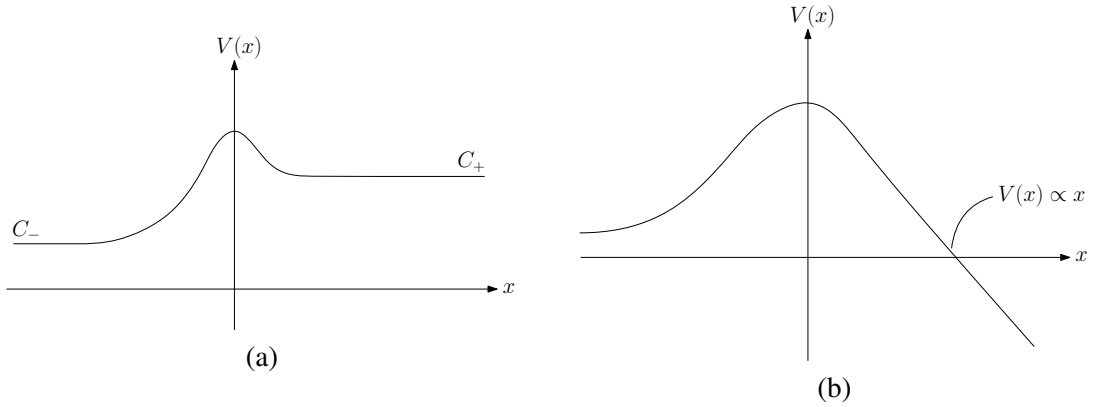


Figure 5.2: Examples of potentials with different asymptotics at $x \to \pm\infty$. Defining the tunneling probability by Eq. (5.17) is still reasonable for such potentials.

the conservation of probability, since, according to Eqs. (5.9), (5.17), R differs from one by an exponentially small quantity which is not caught by the perturbation theory.

The expression (5.17), in fact, does not refer to the asymptotic properties of the potential. Therefore, it maintains its sense in more general cases, for example, when the potential has different constant asymptotics at $x \to \pm\infty$ (figure 5.2 (a)) or even when those asymptotics are not constant (figure 5.2 (b)). Of course, in such cases the WKB method, if applicable at all, gives other expressions for the semiclassical wavefunctions far from the barrier.

5.3 Lifetime of a metastable state

In the previous section we computed the WKB tunneling probability through a potential barrier by considering a steady flux of particles consisting of incident, reflected and transmitted waves. A different problem arises if one takes a potential well separated from the outer region by a barrier and a particle confined initially in the well. The tunneling effect then implies a non-zero probability for the particle to escape the well by penetrating through the barrier. Following the reasoning above, one can write the escape probability per unit time as

$$\frac{dP}{dt} = \frac{|D|^2}{T}\,, \tag{5.20}$$

where the transmission coefficient D is given in Eq. (5.16), and T is the classical period of oscillations of the particle in the well. The important difference between the scattering of particles off the barrier considered before and escaping the potential well is that in the latter case the process is not stationary: the amplitude of particle's wavefunction decreases gradually in the well and increases in the outer region of the potential. This means that the initial state of the particle in the well cannot be an eigenstate of the Hamiltonian with the real eigenvalue. We assume, however, that it is close enough to an eigenstate, so that the probability flux out of the well is suppressed by the width of the barrier and the expression (5.20) for the tunneling probability in the WKB approximation is adequate. Such states are called "metastable".

Eq. (5.20) has limits of applicability. On the one hand, it must be considered at time intervals t much larger than the period of oscillations T. On the other hand, t must not be too large, since otherwise the wavefunction in the well depletes considerably and the flow of probability back to the well may become important. Only at the time scales specified in this way the tunneling probability does not depend on t and is given by Eq. (5.20). Its inverse can then be identified with the lifetime

τ of the metastable state,[1]

$$\tau = \frac{1}{dP/dt} = T|D|^{-2} . \tag{5.21}$$

Let us now approach the problem of decay of a metastable state from the physical perspective. As an example, consider the phenomenon of α-radioactivity. It is known that many nuclei, mainly with atomic numbers $Z \geqslant 84$ and mass numbers $A \geqslant 210$, experience α-decay during which they emit an α-particle ($^4_2$He) and release some energy E_α:

$$^A_Z X \to ^{A-4}_{Z-2} Y + \alpha + E_\alpha . \tag{5.22}$$

The energy E_α is mainly carried by the out-flowing α-particle. It varies in the region $E_\alpha \approx 4 \div 10$ MeV. The lifetime of α-radioactive nuclei varies from $\approx 4 \cdot 10^{-7}$ s for $^{212}_{84}$Po to $\approx 2 \cdot 10^{10}$ years for $^{232}_{90}$Th. On dimensional grounds, one could expect the lifetime to be $\propto E_\alpha^{-1}$. But take, for example, the reaction

$$^{238}_{92}\mathrm{U} \to ^{234}_{90}\mathrm{Th} + \alpha + E_\alpha . \tag{5.23}$$

Here

$$E_\alpha = M_\mathrm{U} - M_\mathrm{Th} - M_\alpha \approx 5 \text{ MeV} , \tag{5.24}$$

and, naively,

$$\tau_{naive} \sim 1 \text{ MeV}^{-1} \sim 10^{-21} \text{ s} , \tag{5.25}$$

which is indeed the characteristic time of processes involving strong nuclear forces. However, the experiment gives

$$\tau_{exp} = 1.4 \times 10^{17} \text{ s} \approx 4.5 \times 10^9 \text{ years} . \tag{5.26}$$

Furthermore, the phenomenological dependence of τ on E_α takes the form (the Geiger-Nuttall law)

$$\log \tau = \frac{B}{\sqrt{E_\alpha}} - A , \tag{5.27}$$

where A and B are the same for different isotopes of one element. Theoretical explanation of Eq. (5.27) and of the striking difference between τ_{naive} and τ_{exp} was given in the framework of quantum theory by Gamov in 1928 and by Gurney and Condon in 1929. The theory of α-decay states that α-particles are formed inside nuclei and that it is energetically favourable for the particle to escape the nucleus, but the potential barrier prevents this.

What does the interaction potential $V(r)$ between an α-particle and a nucleus look like? Outside the nucleus, $r > r_0$, the interaction is determined by the long-range repulsive Coulomb force. Inside the nucleus, $r < r_0$, the short-range strong nuclear force becomes dominant. The latter forms the potential well in which the α-particle is trapped. Overall (see figure 5.3),

$$V(r) = \begin{cases} \infty , & r \leqslant 0 \\ -V_0 , & 0 < r < r_0 \\ \frac{e_N e_\alpha}{r} , & r > r_0 \end{cases} \tag{5.28}$$

[1] For the detailed and accurate discussion of tunneling phenomenon in quantum mechanics and field theory, the interested reader is referred to [3].

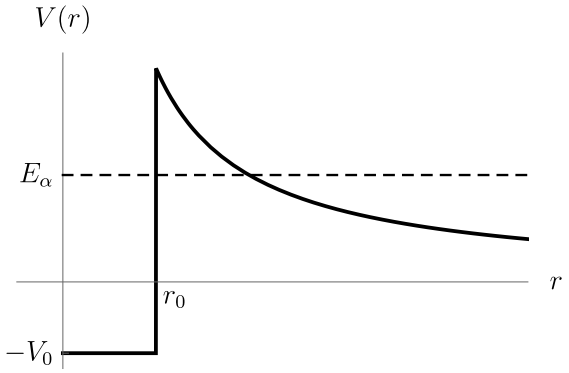


Figure 5.3: The potential between an α-particle and a daughter nucleus.

where V_0 is the binding energy of the α-particle, and q_N and q_α are the electric charges of the nucleus and α-particle respectively. Having this potential, let us compute the lifetime of $^{238}_{92}$U using Eq. (5.21). As a rude estimation, we take

$$T \sim (5\text{ MeV})^{-1} \sim 10^{22}\text{ Hz}\,. \tag{5.29}$$

Next,

$$\begin{aligned} |D|^2 &= \exp\left[-\frac{2}{\hbar}\int_{r_0}^{e_{\rm Th}e_\alpha/E}\sqrt{2m_\alpha\left(\frac{e_{\rm Th}e_\alpha}{x}-E\right)}dx\right] \\ &= \exp\left\{-\frac{2\beta}{\hbar}\sqrt{\frac{2m_\alpha}{E}}\left[\arccos\sqrt{\frac{Er_0}{\beta}}-\sqrt{\frac{Er_0}{\beta}\left(1-\frac{Er_0}{\beta}\right)}\right]\right\}\,, \end{aligned} \tag{5.30}$$

where we denoted $\beta \equiv e_{\rm Th}e_\alpha = \hbar c\alpha N_{\rm TH}N_\alpha$ with $\alpha \approx 1/137$ the fine structure constant, $N_{Th} = 90$ the number of protons in $^{234}_{90}$Th, $N_\alpha = 2$ the number of protons in α-particle. One can simplify this expression by taking $r_0 = 0$ inside the exponent. Then,

$$|D|^2 \approx \exp\left(-\frac{\pi\beta}{\hbar}\sqrt{\frac{2m}{E}}\right) = \exp\left(-\frac{2\pi\beta}{\hbar v}\right)\,, \tag{5.31}$$

where $v = \sqrt{2E_\alpha/m_\alpha}$ is the post-decay velocity of the α-particle. Numerically,

$$\frac{m_\alpha v^2}{2} \sim 5\text{ MeV} \quad\Rightarrow\quad v \approx 0.05c\,, \tag{5.32}$$

hence, $|D|^2 \sim 10^{-71}$. From this and Eq. (5.29) we finally obtain

$$\tau \sim 10^{49}\text{ s}\,. \tag{5.33}$$

This is still off the experimental result (5.26) by about 32 orders of magnitude, the reason being the crudeness of our estimation of the transmission coefficient.

Tunneling out of a metastable state (in field theory it is referred to as false vacuum decay) is one of the phenomena that occur in Nature in a wide range of physical systems. This is an example of a non-perturbative effect, that is, an effect that does not show up when considering small fluctuations around a local minimum of the potential, but is determined by the global structure of the potential. In addendum A we discuss one of the most intriguing applications of the tunneling to particle physics — the decay of the electroweak vacuum.

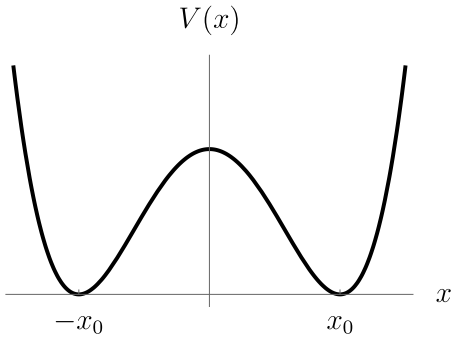


Figure 5.4: A double-well potential.

5.4 Splitting of energy levels in a double-well potential

Consider a one-dimensional potential with two identical minima at $x = \pm x_0$, as shown in figure 5.4. Having a particle confined in either minimum, one could study its bound states neglecting the neighbouring well. This would lead to the conclusion that the states of the particle in the potential are degenerate in energy. However, in one-dimensional quantum systems such degeneracy is impossible (we remind the proof of this in Addendum B). The clue to this issue is that a state describing a particle localized in one of the well of the double-well potential is not a true eigenstate of the Hamiltonian. Indeed, since the potential is parity-symmetric, so is the Hamiltonian and, hence, its eigenstates $\psi(x)$ must be either even, $\psi(-x) = \psi(x)$, or odd $\psi(-x) = -\psi(x)$. To obtain the eigenstates in the WKB approximation, we take a semiclassical wavefunction $\psi_0(x)$ concentrated, say, in the right well, and introduce

$$\psi_1(x) = \frac{1}{\sqrt{2}}(\psi_0(x) + \psi_0(-x)) \,, \quad \psi_2(x) = \frac{1}{\sqrt{2}}(\psi_0(x) - \psi_0(-x)) \,. \tag{5.34}$$

The first of these functions is even, has no nodes and, hence, represents the ground state of the Hamiltonian. The second is odd, has one node at $x = 0$ and represents the first excited state. Our goal is to compute the energy difference $E_2 - E_1$ between ψ_2 and ψ_1 in the leading-order WKB.

According to the Schroedinger equation,

$$\psi_1'' + \frac{2m}{\hbar^2}(E_1 - V)\psi_1 = 0 \,, \quad \psi_2'' + \frac{2m}{\hbar^2}(E_2 - V)\psi_2 = 0 \,. \tag{5.35}$$

Multiplying the first equation by ψ_2, the second — by ψ_1, and taking the difference, we obtain

$$\psi_1''\psi_2 - \psi_2''\psi_1 + \frac{2m}{\hbar^2}(E_1 - E_2)\psi_1\psi_2 = 0 \,. \tag{5.36}$$

Integrating this from 0 to ∞ gives

$$(\psi_1'\psi_2 - \psi_1\psi_2')\big|_0^\infty + \frac{2m}{\hbar^2}(E_1 - E_2)\int_0^\infty \psi_1\psi_2 dx = 0 \,. \tag{5.37}$$

Recall that ψ_1 and ψ_2 are bound states, hence $\psi_1(\infty) = \psi_2(\infty) = 0$. Furthermore, $\psi_2(0) = 0$. Hence, the first term in Eq. (5.37) equals

$$\psi_2'(0)\psi_1(0) = \frac{1}{\sqrt{2}}2\psi_0'(0) \cdot \frac{1}{\sqrt{2}}2\psi_0(0) = 2\psi_0'(0)\psi_0(0) \,. \tag{5.38}$$

On the other hand,

$$\int_0^\infty \psi_1\psi_2 dx = \int_0^\infty \frac{1}{\sqrt{2}}\psi_0 \cdot \frac{1}{\sqrt{2}}\psi_0 dx = \frac{1}{2} \,, \tag{5.39}$$

since ψ_0 is normalized to one. Therefore, Eq. (5.37) becomes

$$2\psi_0(0)\psi_0'(0) + \frac{m}{\hbar^2}(E_1 - E_2) = 0\,. \tag{5.40}$$

Finally, we use the semiclassical expression for the wavefunction $\psi_0(x)$ in the classically forbidden region including the point $x = 0$:

$$\psi_0(x) = \sqrt{\frac{m\omega}{2\pi p}} e^{-\frac{1}{\hbar}\int_x^a dx\,|p|}\,, \tag{5.41}$$

where a is the turning point, $0 < a < x_0$, and we took the normalization constant from Eq. (4.19). Taking the derivative in the leading order WKB approximation,

$$\psi_0'(x) = \frac{p}{\hbar}\psi_0(x), \tag{5.42}$$

we rewrite Eq. (5.40) as

$$\frac{m\omega}{\pi\hbar} e^{-\frac{1}{\hbar}\int_{-a}^a dx\,|p|} + \frac{m}{\hbar^2}(E_1 - E_2) = 0\,. \tag{5.43}$$

Thus,

$$E_2 - E_1 = \frac{\omega\hbar}{\pi} e^{-\frac{1}{\hbar}\int_{-a}^a dx\,|p|}\,. \tag{5.44}$$

Addendum A In quantum field theory tunneling from a metastable state is referred to as the false vacuum decay (see, e.g., chapter 12 of [4]). It happens if the energy functional of a theory contains two non-degenerate local minima, corresponding to two classical vacua, separated by a barrier. Among numerous situations where the decay can occur on practise, one deserves special attention as it concerns with the low-energy electroweak vacuum characteristic for the present-day universe. The fact is that, depending on the values of the various parameters of the Standard Model (in particular, on the value of the top quark Yukawa coupling y_t), the electroweak vacuum may or may not be an absolute minimum of the scalar Higgs potential. For y_t smaller than some critical value $y_{t,crit.}$ it is an absolute minimum and, hence, absolutely stable. For $y_t > y_{t,crit.}$ yet another minimum appears at large magnitudes of the Higgs field (see figure 5.5 for illustration), opening up the possibility for the low-energy vacuum to decay into an energetically more preferable state. The decay of the false vacuum occurs via formation of a bubble of a new phase that starts expanding eating up the old phase. So far it is not clear if y_t is less or larger than $y_{t,crit.}$. However, in any event, the lifetime of the electroweak vacuum in the Standard Model and at the current cosmological epoch exceeds the present age of the universe by many orders of magnitude. Many other directions of research show up if one pursues further the issue of (meta)stability of the electroweak vacuum. Some of them concern with the question of how the lifetime changes when one considers different environment or when one adds new physics at large energy scales.

Addendum B Let us prove that a one-dimensional quantum system cannot have degenerate bound states. Suppose otherwise: there exist ψ_1, ψ_2 such that $\psi_1/\psi_2 \neq$const and

$$H\psi_1 = E\psi_1\,, \quad H\psi_2 = E\psi_2\,. \tag{5.45}$$

From the Schroedinger equation we have

$$\psi_1'' = \frac{2m}{\hbar}(V - E)\psi_1\,, \quad \psi_2'' = \frac{2m}{\hbar}(V - E)\psi_2\,, \tag{5.46}$$

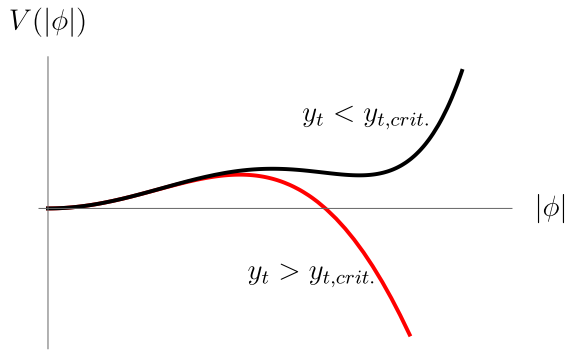


Figure 5.5: Schematic form of the effective Higgs potential at different values of y_t.

hence,

$$\frac{\psi_1''}{\psi_1} = \frac{\psi_2''}{\psi_2} \,, \tag{5.47}$$

or

$$\psi_1''\psi_2 - \psi_1\psi_2'' = 0 \,. \tag{5.48}$$

Integrating this gives

$$\psi_1'\psi_2 - \psi_2'\psi_1 = \text{Const} \,. \tag{5.49}$$

Since ψ_1, ψ_2 are bound states, $\psi_1 \to 0$, $\psi_2 \to 0$, when $x \to \pm\infty$. This means that in Eq. (5.49) Const$= 0$. We conclude that

$$\frac{\psi_1'}{\psi_1} = \frac{\psi_2'}{\psi_2} \,. \tag{5.50}$$

But this can only be true if ψ_1 differs from ψ_2 by a constant multiplier which contradicts the assumption.

▪ **Exercise 5.1 — Restoration of symmetry in the double-well potential.** Consider the symmetric double-well potential of the form

$$V(x) = V_0(x-x_0)^2(x+x_0)^2 \,, \quad V_0 > 0 \,. \tag{5.51}$$

We are interested in the time evolution of the wave function $\Phi(x,t)$ of a particle of mass m, whose energy is well below the barrier separated the wells. Specifically, let the particle be initially localized, say, in the left well,

$$\Phi(x,0) = \psi_0(x) \,, \tag{5.52}$$

where $\psi_0(x)$ denotes the bound state of the left well, and we assume the energy of this state to be much smaller than the height of the barrier. The wave packet (5.52) breaks the parity symmetry of the system. Recall, however, that due to the tunneling phenomenon, the probability to detect the particle in the right well is nonzero at all $t > 0$, and if we wait *sufficiently* long, we should be able to find the particle in either well with almost equal average probabilities. So, the symmetry gets restored in the limit $t \to \infty$, and this exercise is suggested to demonstrate this explicitly.

1. Write the probability $P(x,t)$ to find the particle at the position x and at the time t.
2. Find the explicit expression for the probability $P(t)$ to find the particle in the right well (that is, at $x > 0$).

3. Compute the average probability to find the particle in the right well in the limit of large detection time T:

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T P(t)dt\ . \tag{5.53}$$

▪

▪ **Exercise 5.2 — Perturbation of potential and WKB.** Consider a small time-independent perturbation $\delta V(x)$ of the potential $V(x)$. How does this perturbation affect the semiclassical energy levels of a particle in this potential? Introduce the momenta of the particle in the non-perturbed and perturbed potentials,

$$p_0(x)=\sqrt{2m(E_n-V(x))}\ ,\quad p(x)=\sqrt{2m(E_n+\delta E_n-V(x)-\delta V(x))}\ . \tag{5.54}$$

1. By comparing the quantization conditions for $p_0(x)$ and $p(x)$, find the expression for δE_n in terms of $\delta V(x)$ and $p_0(x)$.
2. Reduce this expression to the form

$$\delta E_n=\frac{1}{T_n}\int_0^{T_n} dt\,\delta V[x_n(t)]\ , \tag{5.55}$$

where T_n denotes the period of oscillations of the particle on the n'th energy level, and $x_n(t)$ is particle's classical trajectory.

▪

▪ **Exercise 5.3 — Rosen-Morse potential.** Recall that one remarkable property of the harmonic oscillator is that its WKB energy spectrum *coincides* with the exact one, despite the formal inapplicability of the LO WKB approach to the energy levels with small n. Here we consider the so-called Rosen-Morse potential (see figure 1),

$$V(x)=-\frac{V_0}{\cosh^2(\frac{x}{x_0})}\ , \tag{5.56}$$

which possesses the same property. Like the harmonic oscillator, this potential is exactly soluble, and the comparison of the exact answer with the result of the LO WKB reveals their coincidence. To make the result more illustrative, let us set

$$x_0=2m=\hbar=1\ ,\quad V_0=\frac{49}{4}\ . \tag{5.57}$$

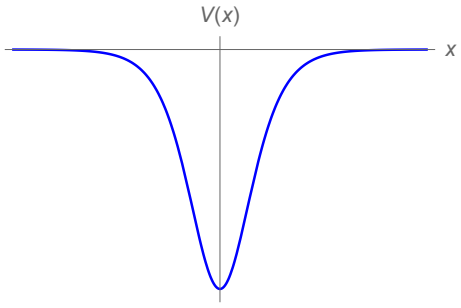


Figure 5.6: The Rosen-Morse potential

1. Find the WKB spectrum of the particle in the potential (5.56), subject to notations (5.57).
   Hint: Computation of the integral $J = \int p dx$ by hand is complicated. Compute instead dJ/dE and then integrate the result. Use the following change of variables,

$$y = \sinh x \,. \tag{5.58}$$

2. Find for which n you can trust the results according to the LO WKB applicability conditions.

▪

▪ **Exercise 5.4 — Tunneling through a parabolic barrier.** Consider a particle with energy E, moving from $x \to -\infty$ towards a potential of the form

$$V(x) = \begin{cases} V_0 \left(1 - \dfrac{x^2}{x_0^2}\right) \,, & |x| < x_0 \\ 0 \,, & |x| > x_0 \,. \end{cases} \tag{5.59}$$

1. Assuming $E < V_0$, find the transmission coefficient of the potential (5.64).
2. For which E you can trust the result of the previous calculation?

▪

▪ **Exercise 5.5 — Lifetime in a cubic potential.** Consider a nonrelativistic particle with mass m and energy E, confined in the well of the potential $V(x) = V_0 x^2(x_0 - x)$, with $V_0 > 0$, $x_0 > 0$.

1. Assuming $E \ll V_0$, find the lifetime of the particle in the well.

▪

▪ **Exercise* 5.6 — Super-WKB approach.** In a variety of problems in Quantum mechanics it is useful to look for the following decomposition of the potential $V = V(x)$,

$$V = W^2 - \frac{\hbar}{\sqrt{2m}} W' \,. \tag{5.60}$$

The function W is called the *superpotential* associated with the potential V. If the superpotential is known, one can build a perturbation theory in $\hbar$ starting from W^2 instead of V. This corresponds to some rearrangement in the series of the original WKB theory. It turns out that for many classes of potentials such rearrangement improves significantly the predictions of the standard WKB.

1. Using eq. (5.60), rewrite the Bohr-Sommerfeld quantization rule in terms of the superpotential and to the LO in $\hbar$.
   Indication: Consider the case when on the turning points, the superpotential takes either opposite ("unbroken SUSY") or equal ("broken SUSY") values.
2. Assuming the oppositve values of the superpotential on the turning points, find the ground state energy E_0.
3. Using the quantization rule found in p.1, compute the energy spectrum of a particle in the "inverse hydrogen atom" potential

$$V(x) = -\frac{1}{x} + \frac{x(x+2)}{(1+x+\frac{1}{2}x^2)^2} + \frac{1}{16} \,, \tag{5.61}$$

   where x is a dimensionless variable, and we put $2m = \hbar = 1$ for simplicity. Compare the answer with the result of the standard LO WKB approximation, and with the exact formula

$$E_n = \frac{1}{16} \frac{n(n+4)}{(n+2)^2} \,, \quad n = 0, 1, 2, \ldots \tag{5.62}$$

   Hint: The superpotential associated with the potential (5.61) is given by

$$W(x) = \frac{x^6 - 16x^4 - 56x^3 - 108x^2 - 240x - 192}{4x(x^2+2x+2)(x^3+6x^2+18x+24)} \,. \tag{5.63}$$

▪

▪ **Exercise* 5.7 — Scattering off the peak.** From the lecture notes we know how to find the transmission and reflection coefficients D and R in the LO WKB approximation and in the case when the energy of an incident particle E is below the height of the barrier V_0. What happens in the limit $E \to V_0$? In this limit, we have only one turning point x_0 of even multiplicity k, such that $V(x_0) = V_0$. Then, in order to match the WKB wave functions to the both sides of the turning point, one has to expand $V(x)$ up to the k'th order around that point.
Let us take for simplicity $x_0 = V_0 = 0$, $k = 2$, and let $V(x)$ approach some constant negative value at $x \to \pm\infty$. Consider the particle with mass m and energy $E < 0$, moving towards x_0 from $x \to -\infty$.

1. Find the region $\mathscr{R}$ of x where it is legitimate both
   (a) to approximate the potential by the first nonzero term of its Taylor expansion around the turning point, and
   (b) to approximate the momentum p by the first two terms of its Taylor expansion in $|E/V(x)|$.
2. Using the approximations found in p.1, write the LO WKB wave functions of the particle in the region $\mathscr{R}$, to the left and to the right sides from the turning point.
3. Now use a path in the region $\mathscr{R}$ continued to the complex plane to connect the LO WKB wave functions found in p.2. Extract the coefficients D and R.
4. Investigate the limit of D and R as $E \to 0$.

▪

▪ **Exercise 5.8 — WKB spectrum of the Hydrogen atom.** Electron levels in the Hydrogen atom are characterized by three quantum number: n_r (the radial number), l (the angular momentum number), and m (the magnetic number). To find the energies of the levels, we consider the Coulomb potential supplemented by a centrifugal term of the form

$$V(r) = -\frac{1}{a_0 M r} + \frac{(l+1/2)^2}{2Mr^2}\,, \tag{5.64}$$

where a_0 is the Bohr radius, M is the electron mass, and we put $\hbar = 1$.

1. Using the WKB approach, find the energy spectrum of an electron in the potential (5.64). Compare with the exact answer.
   Hint: $\int_{x_1}^{x_2} dx \sqrt{\left(1-\frac{x_1}{x}\right)\left(\frac{x_2}{x}-1\right)} = \frac{\pi}{2}(x_1+x_2-2\sqrt{x_1 x_2})$.
2. Compute the energy of the ground state, in eV.
3. What is the degeneracy of the n'th energy level?

▪

▪ **Exercise 5.9 — Pair production in electric field.** Consider the homogeneous electric field of magnitude $\mathscr{E}$, acting in a vacuum (for example, this can be the field between the plates of a vacuum capacitor). Although the notion of "vacuum" implies the absence of any particles, quantum physics, actually, permits the spontaneous creation of electron-positron pairs in the electric field provided that the latter is strong enough. Such creation can be regarded as a tunneling process. Indeed, the energy the system acquires from an electron e^- and a positron e^+ created at the distance x from each other is given by

$$V(x) = 2m_e c^2 - |e|\mathscr{E}x\,, \quad x > 0\,, \tag{5.65}$$

with e the electric charge of the electron, m_e its mass, and c the speed of light. At $x = 0$ the particles disappear, hence one can set $V(0) = 0$. Now, $V(x)$ can be viewed as a potential with the barrier through which the vacuum state is required to tunnel to create one pair.

1. Using the WKB approach, estimate the probability of e^+e^- pair formation in the homogeneous electric field of magnitude $\mathscr{E}$. Compute numerically the value of the magnitude at which this probability becomes of the order of one.
2. Estimate the half-discharge time of a flat vacuum capacitor with the initial charge $Q = 10\,nC$, the plate area $S = 10\,cm^2$, and the plate separation $d = 1\,cm$, due to e^+e^- pair formation in the electric field between the plates.

▪

▪ **Exercise 5.10 — Tunneling in a thermal bath.** Consider a particle confined in the well of a potential and with the ground state energy $E = 0$. Let the potential admit a classically allowed region separated from the well by a barrier of height E_{sph}. Recall that in the WKB approach, the probability for a particle of energy E to escape the well is given by

$$P(E) \sim e^{-B(E)}\,, \quad B(E) = \frac{2}{\hbar}\int_{x_1}^{x_2} |p|\,dx\,, \tag{5.66}$$

where $x_{1,2}$ are the turning points, and p is particle's momentum in the classically forbidden region (see figure 5.10). In our case, the tunneling probability is $P = P(0)$.

Let us now embed the particle into the thermal bath of temperature $T = \beta^{-1}$. Then, one cannot say anymore that particle's energy equals 0. Rather, it becomes distributed according to the Gibbs distribution

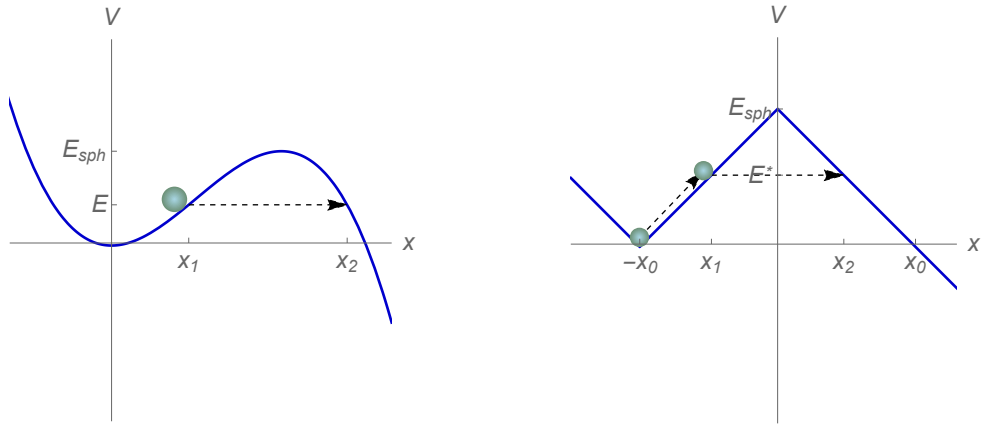
$$G(E) = e^{-\beta E}\,. \tag{5.67}$$

Hence, there appears a probability $\tilde{P}(E)$ to escape the well from *any* energy level, weighted with the expression (5.67). The full tunneling probability P is then obtained by integrating $\tilde{P}(E)$ over energies the particle can have in the well, $0 < E < E_{sph}$.

1. Show that the energy E^* of the most probable energy level from which the particle escapes the well is found by minimizing the expression $\beta E + B(E)$. Having this in mind, write the expression for the full tunneling probability P.
2. Investigate the behavior of P in the large temperature limit, $\beta \to 0$.
3. Compute E^* as a function of β for the barrier of the form (see figure 5.10)

$$V(x) = E_{sph}\left(1 - \left|\frac{x}{x_0}\right|\right)\,, \quad -x_0 < x < x_0\,. \tag{5.68}$$

▪



(a) (b)

Figure 5.7: (a) Tunneling from the level of energy E at zero temperature. (b) Tunneling from the ground level at finite temperature.

III Scattering theory

Lecture 6

> Scattering in non-relativistic classical mechanics; differential and total cross sections; luminosity

6.1 General remarks

The role of the concept of scattering in modern physics is impossible to overestimate. From the theoretical point of view, it is closely related to the idea of *local* interaction between constituents of matter. When the constituents are far apart, that is long before and long after the interaction, they are supposed to move freely. Scattering theory relates these (asymptotically) free initial (in-) and final (out-) states of the system. The direct problem of scattering theory is to compute an out-state as a function of an in-state, provided that the form of the interaction is known. The inverse problem is to deduce the interaction by knowing in- and out-states. The latter situation is normally realised in experiment where in-states are prepared and out-states are detected. The paradigm of local interaction gives access to the real-world physics described in terms of interacting quantum fields. The fact is that, in general, theories with interaction are not solvable. Scattering theory bypasses this circumstance by treating interaction as a small deviation from a free theory. A perturbation theory can, hence, be developed to take into account this deviation in a systematic way.

Needless to say, experiments that probe microscopic structure of matter are mostly scattering experiments. They account for many of the most important discoveries in physics. One can start by mentioning Rutherford's discovery of the atomic nucleus from the scattering of α-particles. Finding elementary particles was also closely related to their scattering properties. For example, Anderson discovered positron and muon by observing their tracks in Wilson chamber. The tracks are chains of droplets in a supersaturated vapor. Their seeds are ions formed due to interaction of energetic particles with molecules of the vapor.

Nowadays, the most prominent scattering experiments are those involving accelerators. In some of them, one collides two beams of particles and observes the result. The examples are LHC (Large Hadron Collider) where the beams of protons are used, its predecessor LEP (Large Electron-Positron collider) where electrons and positron were collided, Tevatron at FNAL (Fermi's national accelerator laboratory) in which protons were collided with antiprotons. Another type of experimental facilities are the ones where a fixed target is used. Here, one can mention neutrino oscillations accelerator experiments. For example, in the linear accelerator in J-PARC (Tokai, Japan) protons are collided with the target material and produce pions (π^+) which decay into antimuons and muon neutrinos. The beam of neutrinos is directed (almost) towards the town of Kamioka 295 km away where the Super-Kamiokande detector is situated. On their way to the detector, neutrino

oscillate (change their flavor). By registering decay products of resulting neutrinos in the detector, one infers how strong different neutrino flavors are mixed.

Non-accelerating particle scattering is also present on the current physics frontier. Perhaps, the most exciting example here is dark matter direct detection experiments. Elastic scattering of hypothetical dark matter particles on nuclei of a detector material would produce a nuclear recoil that one can hope to register. For example, Weakly Interacting Massive Particles (WIMPs) of masses 10 to 10^3 GeV are expected to produce recoils in the range 1 to 100 keV [5]. The very incomplete list of experiments currently at work includes DAMA/LIBRA, SuperCDMS, CRESST, EDELWEIS, DRIFT.

In the next four lectures we will discuss scattering in non-relativistic quantum physics. One may fairly expect that many notions of scattering theory can be inherited from classical mechanics. Because of this, in this lecture we collect few basic facts about classical scattering. Next, one expects that when the limit $\hbar \to 0$ is properly taken, quantum observables (such as the differential cross section) reduce to their classical analogs, while in general the results (and the methods of obtaining them) are different. It is worth to note here that the perturbation theory, to which the major part of the reminder of these notes is devoted, is based on having a small *interaction constant*, not small $\hbar$ as it was before. Therefore, we do not expect the coincidence in the results of quantum and classical calculations. There are lucky exceptions, however. For example, the Rutherford's formula for the (non-relativistic) scattering in the Coulomb field,

$$\frac{d\sigma}{d\Omega} = \left(\frac{Z_1 Z_2 e^2}{2mv^2}\right)^2 \frac{1}{\sin^4 \frac{\theta}{2}} , \tag{6.1}$$

happens to be the same both in quantum and classical theory. Rutherford himself used the classical formula, and if it had not been for this coincidence, who knows for how long the discovery of the nucleus would have been delayed.

6.2 Non-relativistic classical scattering

Consider a point particle of mass m moving in the potential $V(x)$. Assume that the potential vanishes fast enough as $|x| \to \infty$, so that at $t \to \pm\infty$ the particle moves freely:

$$\begin{aligned} \mathbf{x}(t \to -\infty) &= \mathbf{x}_{\text{in}} + \mathbf{v}_{\text{in}} t \\ \mathbf{x}(t \to +\infty) &= \mathbf{x}_{\text{out}} + \mathbf{v}_{\text{out}} t \ . \end{aligned} \tag{6.2}$$

These formulas specify the initial and final states of the particle. Scattering theory concerns with determining $\mathbf{x}_{\text{out}}$ and $\mathbf{v}_{\text{out}}$ as functions of $\mathbf{x}_{\text{in}}$ and $\mathbf{v}_{\text{in}}$. To do this, it is sufficient to find a general solution of Newton's equation

$$m\ddot{\mathbf{x}} = -\frac{dV}{d\mathbf{x}} , \tag{6.3}$$

select a particular solution satisfying the first of Eqs. (6.2) for fixed values of $\mathbf{x}_{\text{in}}$ and $\mathbf{v}_{\text{in}}$ and see if it also satisfies the second of Eqs. (6.2) with some $\mathbf{x}_{\text{out}}$ and $\mathbf{v}_{\text{out}}$.

In general, not all trajectories possess asymptotics (6.2). For example, any periodic motion and, more generally, any motion that happens in a finite region of space does not exhibit such asymptotic behavior. Planets orbiting a star are an obvious example. Next, it may happen that not all initial states characterised by some $\mathbf{x}_{\text{in}}$, $\mathbf{v}_{\text{in}}$ evolve into a final state described by some $\mathbf{x}_{\text{out}}$, $\mathbf{v}_{\text{out}}$. The particle may be captured by the potential well and stay there forever or it may fall at the scattering center in a finite time. Both options are possible, for example, for the gravitational potential created by a black hole.

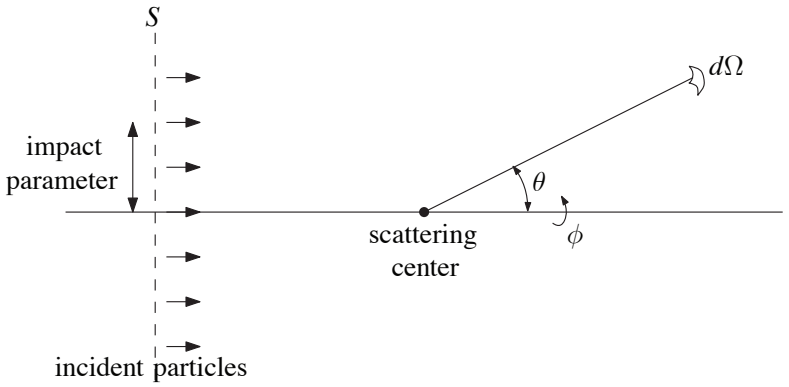


Figure 6.1: Illustration for the definition of cross section.

The quantity of the main interest in scattering theory is a (differential) cross section. Consider a steady homogeneous flux of particles approaching the scattering center as shown in Fig. 6.1. Define the number density n as a number of particles crossing the plane perpendicular to the flux, per unit area per unit time. Then, in CGS units

$$n = \text{const} \cdot \frac{1}{\text{cm}^2 \cdot \text{s}} \,. \tag{6.4}$$

Let dN/dt be the number of particles scattered in a direction determined by θ, ϕ, within the solid angle $d\Omega = d\cos\theta d\phi$, per unit time. Then,

$$\frac{dN}{dt} = \frac{d\sigma}{d\Omega} n \, d\Omega \,. \tag{6.5}$$

The quantity $d\sigma/d\Omega$ is called the differential cross section. Since the units of n are $\text{cm}^{-2}\text{s}^{-1}$, and the units of dN/dt are s^{-1}, we have

$$\frac{d\sigma}{d\Omega} = \text{const} \cdot \text{cm}^2 \,. \tag{6.6}$$

The total cross section σ is obtained by integrating $d\sigma/d\Omega$ over all possible scattering directions,

$$\sigma = \int \frac{d\sigma}{d\Omega} \, d\Omega \,. \tag{6.7}$$

The total cross section is effectively an area of influence of the scattering potential on the incident particles. For example, the cross section of a solid ball of radius r is simply given by $\sigma = \pi r^2$. A more complicated example is the scattering of point-like charged particles by the Coulomb field of a fixed target particle. The Coulomb potential,

$$V(r) = \frac{\alpha}{r} \,, \tag{6.8}$$

is attractive, $\alpha < 0$, if the charges of the incident particles and the target are opposite, and repulsive, $\alpha > 0$, otherwise. Computing the differential cross section yields Eq. (6.1) in which $Z_1 e$ and $Z_2 e$ are the charges of the scattering center and the scattered particles, and v is the initial velocity of the particles, see Exercise 6.1.

The scattering of two particles on each other can be viewed as the scattering of one particle on a potential $V(|\mathbf{x}_1 - \mathbf{x}_2|)$ generated by the particles separated by the distance $|\mathbf{x}_1 - \mathbf{x}_2|$. Indeed, consider the equations of motion of the two particles,

$$m_1 \ddot{\mathbf{x}}_1 = -\frac{\partial V}{\partial \mathbf{x}_1} \,, \quad m_2 \ddot{\mathbf{x}}_2 = -\frac{\partial V}{\partial \mathbf{x}_2} \,. \tag{6.9}$$

Introduce the relative distance $\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2$, and the position of the center of the mass $\mathbf{X}$,

$$\mathbf{X} = \frac{m_1\mathbf{x}_1 + m_2\mathbf{x}_2}{m_1 + m_2} \,. \tag{6.10}$$

Then, one can rewrite Eqs. (6.9) as

$$m_{\text{eff}}\ddot{\mathbf{x}} = -\frac{\partial V}{\partial \mathbf{x}} \,, \quad \ddot{\mathbf{X}} = 0 \,, \quad m_{\text{eff}} = \frac{m_1 m_2}{m_1 + m_2} \,. \tag{6.11}$$

The first of these equations is solved trivially, while the second describes the scattering of the particle of mass m_{eff} on the potential $V(|\mathbf{x}_1 - \mathbf{x}_2|)$.

While the total cross section is a frame-independent quantity, the differential cross section depends on the reference frame in which it is computed. The two reference frames most commonly used on practice are

- the laboratory frame in which there is an incident particle with a non-zero initial momentum and a target particle with zero initial momentum,
- the center-of-mass frame in which both particles have non-zero momentum, but their sum (the total momentum) is zero.

The relation between the differential cross sections written in these two frames is the following (see Exercise 6.2)

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{lab}} = \left(\frac{d\sigma}{d\Omega}\right)_{\text{cm}} \frac{\left(1 + 2\lambda\cos\theta_{\text{cm}} + \lambda^2\right)^{3/2}}{1 + \lambda\cos\theta_{\text{cm}}} \,, \tag{6.12}$$

where $\lambda = m_1/m_2$ and θ_{cm} is the scattering angle in the center-of-mass frame.

Finally, let us mention one quantity which is an important characteristic of accelerators. The rate dN/dt of events of a particular kind (e.g., the Higgs boson production rate via the reaction $p + p \to H + \text{anything}$) is given by

$$\frac{dN}{dt} = L \cdot \sigma \,, \tag{6.13}$$

where σ is the cross section of the particular channel we are interested in, and L is called luminosity. In CGS units, its dimension is $\text{cm}^{-2}\text{s}^{-1}$. For example, the designed luminosity of the LHC is 10^{34} $\text{cm}^{-2}\text{s}^{-1}$. One also considers integrated luminosity defined as an integral of L over time.

▪ **Exercise 6.1 — Classical scattering on a Coulomb potential.** Consider a constant flux of non-interacting particles (i.e. a constant number of n particles per area and time) of mass m with fixed energy and direction approaching a central potential $U(r)$ (a scattering center).

1. Show that the orbit equation for each individual particle is given by (see figure 6.2)

$$\phi(r) = \int_{\infty}^{r} \frac{L/r'^2 dr'}{\sqrt{2m(E - U(r')) - L^2/r'^2}} \,, \tag{6.14}$$

   with E the energy and L the angular momentum. For the Coulomb potential $U(r) = \alpha/r$ with $\alpha \in$ Reals and for $E > 0$ this is a scattering orbit (a hyperbola).
2. Use the previous equation to determine the deflection angle θ for a particle starting at $r = \infty$ and going back to $r = \infty$.

   Hint: Use the formula

$$\int \frac{dx}{x\sqrt{ax^2 + bx + c}} = \frac{1}{\sqrt{-c}} \arcsin \frac{bx + 2c}{x\sqrt{b^2 - 4ac}} \,. \tag{6.15}$$

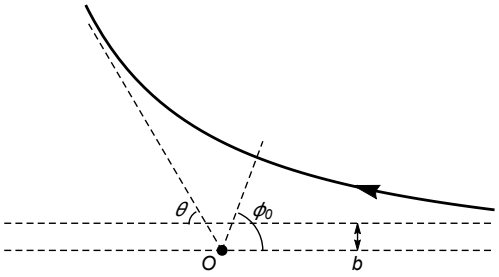


Figure 6.2: The Coulomb potential

3. Replace the constants of motion (E,L) by (E,b), with b the impact parameter, i.e. the normal distance between the asymptote of the incident particle and the scattering center at $r=0$.
4. Determine the number of particles dN per area and per time in a ring between b and $b+db$. If there is a one-to-one functional relation $b(\theta)$ between b and the scattering angle, then dN is at the same time the number of particles that is scattered in an angle between θ and $\theta+d\theta$. Use this to show that the differential cross section for a Coulomb scattering (i.e. the Rutherford scattering formula) is given by

$$\frac{d\sigma}{d\Omega} = \frac{\alpha^2}{16E^2}\frac{1}{\sin^4\frac{\theta}{2}} \,. \tag{6.16}$$

5. Show that the total cross section is infinite. Interpret the result.

▪

▪ **Exercise 6.2 — Differential cross section transformation.** Consider a particle of mass m_1 scattering off a target particle of mass m_2 in the non-relativistic limit.

1. Show that the relation between the differential cross section in the laboratory frame at a given lab angle θ_{lab} and the differential cross section in the center of mass frame at the corresponding angle θ_{cm} can be written as

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{lab}} = \frac{\left(1+2\lambda\cos\theta_{cm}+\lambda^2\right)^{3/2}}{|1+\lambda\cos\theta_{cm}|}\left(\frac{d\sigma}{d\Omega}\right)_{\text{cm}} \tag{6.17}$$

with $\lambda = m_1/m_2$ the mass ratio of the two particles.

Hint: Show that the relation between $\cos\theta_{\text{lab}}$ and $\cos\theta_{\text{cm}}$ is given by

$$\cos\theta_{\text{lab}} = \frac{\cos\theta_{\text{cm}}+\lambda}{(1+2\lambda\cos\theta_{\text{cm}}+\lambda^2)^{1/2}} \,. \tag{6.18}$$

▪

Lecture 7

> Møller operators; S-matrix; S-matrix in terms of evolution operator in the interaction picture; properties of S-matrix and Møller operators; S-matrix and energy conservation; S-matrix and the scattering amplitude.

7.1 Møller operators and S-matrix

In this lecture, we formulate the scattering problem in non-relativistic quantum mechanics. In going from classical to quantum description, one replaces particle's trajectories by states $|\psi(t)\rangle$ in the Hilbert space $\mathscr{H}$, which evolve in time according to the Schroedinger equation

$$-\frac{\hbar}{i}\frac{\partial|\psi(t)\rangle}{\partial t} = H|\psi(t)\rangle\ . \tag{7.1}$$

We take the Hamiltonian in the form

$$H = H_0 + V\ ,\quad H_0 = \frac{p^2}{2m}\ , \tag{7.2}$$

where H_0 is the free particle Hamiltonian, and V is the potential (interaction) term. The solution of Eq. (7.1) is

$$|\psi(t)\rangle = U(t)|\psi_0\rangle\ ,\quad U(t) = e^{-\frac{i}{\hbar}Ht}\ . \tag{7.3}$$

Here $U(t)$ is the evolution operator, and $|\psi_0\rangle$ is an arbitrary state in $\mathscr{H}$, which specifies the initial conditions for $|\psi(t)\rangle$.

In what follows, it will be convenient to omit $\hbar$ in calculations. To do this, we adopt the system of units called natural, in which $\hbar = 1$. If one measures energy in eV, then setting $\hbar$ to one amounts to setting a unit of time to $\approx 0.7\cdot 10^{-15}$ s (see Exercise 7.1).

We now want to make analogy with Eqs. (6.2). Assume the potential $V(x)$ to fall off fast enough at $|\mathbf{x}|\to\infty$ (the precise conditions will be given below). Then one can expect the time-evolving state $|\psi(t)\rangle$ to behave in the remote past and future as if it was governed by the evolution operator of the free Hamiltonian:

$$\begin{aligned}&|\psi(t)\rangle \to U_0(t)|\psi_{\text{in}}\rangle\ ,\quad t\to-\infty\\ &|\psi(t)\rangle \to U_0(t)|\psi_{\text{out}}\rangle\ ,\quad t\to\infty\end{aligned} \tag{7.4}$$

for some $|\psi_{\text{in}}\rangle$ and $|\psi_{\text{out}}\rangle$. Here the convergence is assumed with respect to the norm in $\mathscr{H}$,

$$|\psi(t)\rangle \to |\phi(t)\rangle\ ,\ t\to t_0\ \ \Leftrightarrow \||\psi(t)-\phi(t)\rangle\|\to 0\ ,\ t\to t_0\ . \tag{7.5}$$

The states $|\psi_{\rm in}\rangle$ and $|\psi_{\rm out}\rangle$ specify the asymptotically free evolution of the wave packet in the same way as $\mathbf{x}_{\rm in}$, $\mathbf{v}_{\rm in}$ and $\mathbf{x}_{\rm out}$, $\mathbf{v}_{\rm out}$ specify the asymptotically free motion of a classical particle far from the scattering center. The direct problem of scattering theory is to find $|\psi_{\rm out}\rangle$ as a function of $|\psi_{\rm in}\rangle$. As a first step in this direction, let us find an operator relating the two states. To this end, we rewrite Eq. (7.3) and use the second of Eqs. (7.4) to get

$$|\psi_0\rangle = U^\dagger(t)|\psi(t)\rangle = \lim_{t\to\infty} U^\dagger(t)U_0(t)|\psi_{\rm out}\rangle \equiv \Omega_-|\psi_{\rm out}\rangle \,. \tag{7.6}$$

Similarly,

$$|\psi_0\rangle = U^\dagger(t)|\psi(t)\rangle = \lim_{t\to-\infty} U^\dagger(t)U_0(t)|\psi_{\rm in}\rangle \equiv \Omega_+|\psi_{\rm in}\rangle \,. \tag{7.7}$$

Combining the two formulas gives

$$|\psi_{\rm out}\rangle = \Omega_-^\dagger\,\Omega_+|\psi_{\rm in}\rangle \equiv S|\psi_{\rm in}\rangle \,. \tag{7.8}$$

The operators Ω_- and Ω_+ are called Møller operators, and the operator S is called the scattering matrix or, simply, the S-matrix.

The S-matrix can be conveniently expressed through the evolution operator in the so-called interaction (or Dirac) picture. In this picture, a state is written as

$$|\psi_I(t)\rangle = e^{iH_0t}|\psi(t)\rangle = e^{iH_0t}e^{-iHt}|\psi_0\rangle \,. \tag{7.9}$$

In other words, we trace only the part of the evolution provided by the interaction part of the Hamiltonian H. An operator O_S in the Schroedinger picture is related to that in the interaction picture via

$$O_I = e^{iH_0t}O_s e^{-iH_0t} \,. \tag{7.10}$$

From Eqs. (7.9) and (7.4) we see that

$$|\psi_{\rm in}\rangle = \lim_{t\to-\infty}|\psi_I(t)\rangle \,, \quad |\psi_{\rm out}\rangle = \lim_{t\to\infty}|\psi_I(t)\rangle \,. \tag{7.11}$$

Let us write Eq. (7.9) at two moments of time $t_1 > t_2$:

$$|\psi_I(t_1)\rangle = e^{iH_0t_1}e^{-iHt_1}|\psi_0\rangle \,, \quad |\psi_I(t_2)\rangle = e^{iH_0t_2}e^{-iHt_2}|\psi_0\rangle \,. \tag{7.12}$$

Eliminating $|\psi_0\rangle$ gives

$$\psi_I(t_1) = e^{iH_0t_1}e^{-iHt_1}e^{iHt_2}e^{-iH_0t_2}|\psi_I(t_2)\rangle \equiv S(t_1,t_2)|\psi_I(t_2)\rangle \,. \tag{7.13}$$

We see that the evolution operator in the interaction picture is given by

$$S(t_1,t_2) = e^{iH_0t_1}e^{iH(t_2-t_1)}e^{-iH_0t_2} \,. \tag{7.14}$$

Comparing with Eq. (7.8), we obtain

$$S = \lim_{t_1\to+\infty}\lim_{t_2\to-\infty} S(t_1,t_2) \,. \tag{7.15}$$

That is, the S-matrix is a limit of the evolution operator in the interaction picture.

7.2 Properties of S-matrix and Møller operators

Recall that an operator U acting in the Hilbert space $\mathscr{H}$ is called unitary if
(*i*) The domain $D(U)$ of U is the full Hilbert space, $D(U) = \mathscr{H}$;
(*ii*) The range $R(U)$ of U is again the full Hilbert space, $R(U) = \mathscr{H}$;
(*iii*) U preserves the norm of the vectors, $\||U\psi\rangle\| = \||\psi\rangle\|$.

By the definition, the Møller operators and the S-matrix are limits of sequences of unitary operators. It is natural to ask if these limits are themselves unitary operators. It turns out that this is not always the case but the conditions under which $\Omega_\pm$ are unitary can be well understood from the physical point of view. To work out these conditions, we need first the relations

$$H\Omega_\pm = \Omega_\pm H_0 \ , \quad H_0\Omega_\pm^\dagger = \Omega_\pm^\dagger H \ . \tag{7.16}$$

The second relation is obtained from the first by taking the hermitian conjugate. The proof of the first relation goes as follows,

$$\begin{aligned} U^\dagger(\tau)\Omega_\pm &= U^\dagger(\tau)\lim_{t\to\mp\infty} U^\dagger(t)U_0(t) \\ &= \lim_{t\to\mp\infty} U^\dagger(\tau)U^\dagger(t)U_0(t)U_0(\tau)U_0^\dagger(\tau) \\ &= \lim_{t\to\mp\infty} U^\dagger(t+\tau)U_0(t+\tau)U_0^\dagger(\tau) \\ &= \Omega_\pm U_0^\dagger(\tau) \ . \end{aligned} \tag{7.17}$$

Taking the derivative of the both parts with respect to τ and setting τ to zero, we arrive at the first of Eqs. (7.16). Consider now the eigenvectors of the unperturbed Hamiltonian H_0, which are momentum eigenstates $|\mathbf{p}\rangle$ with the eigenvalues $E_p = \mathbf{p}^2/2m$. We have

$$H\Omega_+|\mathbf{p}\rangle = \Omega_+ H_0|\mathbf{p}\rangle = E_p\Omega_+|\mathbf{p}\rangle \ . \tag{7.18}$$

That is, $\Omega_+|\mathbf{p}\rangle$ are eigenvectors of the full Hamiltonian H with the eigenvalues E_p. Since $|\mathbf{p}\rangle$ form a complete set of states in $\mathscr{H}$, the above shows that $D(\Omega_+) = \mathscr{H}$. However, in general, $R(\Omega_+) \neq \mathscr{H}$, as Ω_+ maps all vectors into the eigenstates of H with positive eigenvalues. If H has negative eigenvalues, Ω_+ is not unitary. This arguments can be repeated also for Ω_-. But negative eigenvalues of H are associated with bound states.[1] Thus, we conclude that if the potential V admits bound states, the Møller operators are not unitary.

Operators for which the conditions (i) and (iii) are satisfied, but the condition (ii) is violated, are called *isometric*. It is easy to provide an example of such operator in an infinite-dimensional vector space with the basis labelled by integers: $|1\rangle$, $|2\rangle$, ..., $|n\rangle$, ... Let U act as a shifting operator on this basis, $U|n\rangle = |n+1\rangle$ for all $n \geqslant 1$. Since $|n\rangle$ form a basis, this defines the action of U in the whole vector space. Clearly, the conditions (i) and (iii) are satisfied in this case, but there are no vectors mapped by U into $|1\rangle$, hence the range of U does not coincide with its domain. Note that the situation we have just described is not possible in a finite-dimensional space as you are asked to prove in Exercise 7.3.

Bound states of H are analogous to closed trajectories in classical scattering considered in the previous lecture. Together with the scattering states, they form a complete set of eigenstates of the full Hamiltonian H. Next, it is easy to see that subspaces of bound and scattering states are, actually, orthogonal to each other. Indeed, let $|\psi_1\rangle$ lie in the space of scattering states, and $|\psi_2$ lie

[1] It is actually possible to construct potentials which admit positive-energy bound states. Hence, for them energy spectra of scattering and bound states are mixed up. All such potentials are, however, quite involved, and we will not consider them here. See, e.g., section III4 of [6].

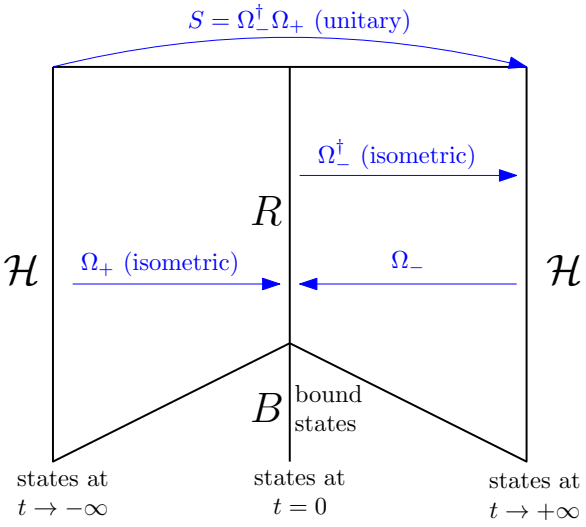


Figure 7.1: Illustration of the domains and ranges of $\Omega_\pm$ in presence of bound states.

in the space of bound states. We can decompose $|\psi_1\rangle$ and $|\psi_2\rangle$ into the eigenstates of H with the positive and negative eigenvalues accordingly:

$$\begin{aligned} |\psi_1\rangle &= \sum c_n |\psi_n\rangle \,, \quad H|\psi_n\rangle = E_n|\psi_n\rangle \,, \quad E_n > 0 \,, \\ |\psi_2\rangle &= \sum \tilde{c}_m |\tilde{\psi}_m\rangle \,, \quad H|\tilde{\psi}_m\rangle = \tilde{E}_m|\tilde{\psi}_m\rangle \,, \quad \tilde{E}_m < 0 \,. \end{aligned} \tag{7.19}$$

Since $\langle\psi_n|\tilde{\psi}_m\rangle = 0$ for all n and m, we have $\langle\psi_1|\psi_2\rangle = 0$. Therefore, one can write

$$\mathscr{H} = R(\Omega_+) \bigoplus B \,, \tag{7.20}$$

where B denotes the subspace spanned by the bound states. This situation is illustrated in figure 7.1.

The fact that the Møller operators are non-unitary does not imply that the S-matrix is also non-unitary. Indeed, under a quite natural assumption that

$$R(\Omega_-) = R(\Omega_+) \,, \tag{7.21}$$

from figure 7.1 we see that $R(S) = \mathscr{H} = D(S)$ and all three conditions in the definition of a unitary operator are satisfied. The fundamental problem of scattering theory is to determine "asymptotic conditions" under which both

- the Møller operators are well defined (in our case this means that the asymptotic behaviour of the full Hamiltonian's wavefunction can be correctly approximated by the free Hamiltonian's wavefunction), and
- the S-matrix is unitary (or, equivalently, the condition (7.21) holds).

The asymptotic conditions can be translated into the requirements on the potential V. For simplicity, below we will discuss spherically-symmetric potentials, $V = V(r)$. Then, the sufficient requirements are the following (see section 2-c of [7] for the proof),

- $\lim_{r\to\infty} V(r) \propto O\left(r^{-\alpha}\right)$ with $\alpha > 3$,
- $\lim_{r\to 0} V(r) \propto O\left(r^{-\beta}\right)$ with $\beta < 3/2$, and
- V is a continuous function of r.

Most of the potentials of physical interest satisfy these requirements. But, for example, the Coulomb potential does not obey them, since it does not fall off fast enough at infinity. It provides an example of a long-ranged interaction, so that a particle "feels" the scattering center no matter how far it is from the latter. The instructive way to see this is to integrate Eq. (6.1) over the solid angle, see

Exercise 6.1. It is worth noting that the scattering theory can actually be generalized to encompass more general potentials than those obeying the conditions above and, in particular, the Coulomb potential. But this involves redefinition of the Møller operators in a more general form, which will not be discussed here.

7.3 S-matrix and the scattering amplitude

In classical elastic scattering energy conservation prescribes kinetic energies of a particle to be the same long before and long after the interaction. In quantum physics, conservation laws are inferred from commutators of the corresponding operator with the Hamiltonian. We have,

$$\begin{aligned}[H_0,S] &= H_0S - SH_0 = H_0\Omega_-^\dagger\Omega_+ - \Omega_-^\dagger\Omega_+H_0 \\ &= \Omega_-^\dagger H\Omega_+ - \Omega_-^\dagger\Omega_+H_0 = \Omega_-^\dagger\Omega_+H_0 - \Omega_-^\dagger\Omega_+H_0 = 0\,,\end{aligned} \tag{7.22}$$

where Eqs. (7.8) and (7.16) were used. This result expresses the conservation of energy in a scattering experiment. Indeed, the energy of the in (out)-state is associated with the matrix element $\langle\psi_{\rm in}|H_0|\psi_{\rm in}\rangle$ ($\langle\psi_{\rm out}|H_0|\psi_{\rm out}\rangle$), and, due to Eq. (7.22),

$$\langle\psi_{\rm out}|H_0|\psi_{\rm out}\rangle = \langle\psi_{\rm in}|S^\dagger H_0 S|\psi_{\rm in}\rangle = \langle\psi_{\rm in}|H_0|\psi_{\rm in}\rangle\,. \tag{7.23}$$

It is natural to choose the eigenstates of the free Hamiltonian $|\mathbf{p}\rangle$ as a basis with respect to which one computes the matrix elements of the S-matrix. The matrix element $\langle\mathbf{p}'|S|\mathbf{p}\rangle$ defines a probability amplitude for the momentum state $|\mathbf{p}\rangle$ to be scattered into the state $|\mathbf{p}'\rangle$. Although it does not correspond to any physically reliable process (in practice, one deals with wave packets rather than momentum eigenstates), one can use it to relate $\psi_{\rm out}$ to $\psi_{\rm in}$:

$$\psi_{\rm out}(\mathbf{p}') = \int d^3\mathbf{p}\langle\mathbf{p}'|S|\mathbf{p}\rangle\,\psi_{\rm in}(\mathbf{p})\,. \tag{7.24}$$

The conservation of energy in a scattering process allows us to write

$$\langle\mathbf{p}'|S|\mathbf{p}\rangle = \delta(E_{p'}-E_p)\times \text{ some function of } \mathbf{p} \text{ and } \mathbf{p}'\,. \tag{7.25}$$

Note also that in the absence of interaction $S=1$. Hence, it is convenient to write

$$S = 1 + R\,, \tag{7.26}$$

where $[H_0,R]=0$. In more details,

$$\begin{aligned}\langle\mathbf{p}'|S|\mathbf{p}\rangle &= \delta^{(3)}\left(\mathbf{p}'-\mathbf{p}\right) - 2\pi i\delta(E_{p'}-E_p)\,t(\mathbf{p}'\leftarrow\mathbf{p}) \\ &= \delta^{(3)}\left(\mathbf{p}'-\mathbf{p}\right) + \frac{i}{2\pi m}\delta(E_{p'}-E_p)\,f(\mathbf{p}'\leftarrow\mathbf{p})\,.\end{aligned} \tag{7.27}$$

Here the function t represents matrix elements of the T-matrix, to be introduced later, and the function f is called the scattering amplitude. Eqs. (7.27) are the simplest example of the so-called cluster decomposition: the first terms in the r.h.s. of them correspond to the absence of scattering, and the second — to the genuine scattering process.[2] As we will see in the next lecture, the scattering amplitude is simply related to the quantum differential cross section: it turns out that

$$\frac{d\sigma}{d\Omega} = |f|^2\,. \tag{7.28}$$

[2]Note that one cannot write the S-matrix in this form for, say, the Coulomb potential, as the latter produces the long-ranged force for which the non-scattering events are impossible.

▪ **Exercise 7.1 — Natural units.** Check that in the system of units in which the energy is measured in eV, and $\hbar = 1$, the unit of time corresponds to $\approx 0.7 \cdot 10^{-15}$ s. ▪

▪ **Exercise 7.2 — Interaction picture.** Consider a system with the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$, where $\hat{H}_0$ is the free Hamiltonian and $\hat{V}$ is the interaction. Define the interaction picture for states and operators via the relations

$$\begin{aligned} \Psi_I(t) &= \hat{U}_0^\dagger(t)\Psi_S(t)\,, \\ \hat{A}_I(t) &= \hat{U}_0^\dagger(t)\hat{A}_S\hat{U}_0(t)\,, \end{aligned} \tag{7.29}$$

where $\hat{U}_0(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}$, and the subscript S denotes quantities in the Schrodinger picture.

1. Find the relation between the states and operators in the interaction and Heisenberg pictures.
2. Show that the evolution of the wave function in the interaction picture is described by the interaction term $\hat{V}$ in the same picture, i.e.

$$-\frac{\hbar}{i}\frac{d}{dt}\Psi_I(t) = \hat{V}_I\Psi_I(t)\,. \tag{7.30}$$

3. Express the evolution operator in the interaction picture $\hat{U}_I(t)$ through $\hat{U}(t)$ and $\hat{U}_0(t)$. Find a differential equation which $\hat{U}_I(t)$ obeys and determine the initial condition for it.

▪

▪ **Exercise 7.3 — Unitarity versus isometry.** Recall that the operator $\hat{U}$ acting in the Hilbert space $\mathscr{H}$ is called unitary if

$$\mathscr{D}(\hat{U}) = \mathscr{H}\,, \quad \mathscr{R}(\hat{U}) = \mathscr{H}\,, \quad \hat{U}^\dagger\hat{U} = 1\,, \tag{7.31}$$

where the last equality should be understood in the operator sense,

$$\langle\Phi|\hat{U}^\dagger\hat{U}|\Phi\rangle = \langle\Phi|\Phi\rangle = 1\,, \quad \forall\Phi \in \mathscr{H}\,. \tag{7.32}$$

1. Prove that the set of conditions (7.31) is equivalent to the following set,

$$\mathscr{D}(\hat{U}) = \mathscr{H}\,, \quad \hat{U}^\dagger\hat{U} = 1\,, \quad \hat{U}\hat{U}^\dagger = 1\,. \tag{7.33}$$

2. Prove that if $\mathscr{H}$ is finite-dimensional, the conditions (7.33) can be eased to

$$\mathscr{D}(\hat{U}) = \mathscr{H}\,, \quad \hat{U}^\dagger\hat{U} = 1\,. \tag{7.34}$$

3. Assuming $\mathscr{H}$ to be infinite-dimensional and with the basis $|1\rangle$, $|2\rangle$, ..., $|n\rangle$,... , construct the sequence of unitary operators $\hat{U}(\lambda)$ such that $\lim_{\lambda\to 0}\hat{U}(\lambda) = \hat{\Omega}$, where $\hat{\Omega}$ is an isometric non-unitary operator.

▪

▪ **Exercise 7.4 — Semiclassical S-matrix in one dimension.** Consider a one-dimensional potential barrier located around the point $x = 0$. Assume that at large $|x|$, the potential falls off fast enough to ensure the plane wave asymptotic solutions of the Schroedinger equation. Let $|\Psi_{in}\rangle$ be the state representing a localized right-moving wave packet at large negative x and at the moment of time $-T$. We are interested in how this wave packet transforms as it scatters off the barrier. Denote by $|\Psi_{out}\rangle$ the state representing the packet transmitted through the barrier in the region of large positive x and at the moment of time T. Then, one can define the operator $\hat{S}$ such that

$$\hat{S}|\Psi_{in}\rangle = |\Psi_{out}\rangle\,. \tag{7.35}$$

1. With the transmission coefficient of the barrier given by

$$D(p) = \mathrm{Tanh}^2(p/p_0) \,, \tag{7.36}$$

compute the matrix elements of $\hat{S}$ in the space of Gaussian functions,

$$S(p', \sigma'; p, \sigma) \equiv \langle \Psi_{p',\sigma'} | \hat{S} | \Psi_{p,\sigma} \rangle \,, \quad \Psi_{p,\sigma}(x) = C_{p,\sigma} e^{-\frac{x^2}{4\sigma^2}} \,, \tag{7.37}$$

where $C_{p,\sigma}$ is the appropriate normalization constant (see Exercise 1.2).

▪

Lecture 8

Optical theorem; cross section and scattering amplitude; Møller operators via the Green's function.

8.1 Optical theorem

The optical theorem relates imaginary part of the scattering amplitude in the forward direction, $\mathrm{Im}\, f(\mathbf{p} \leftarrow \mathbf{p})$, with the total cross section of the scattering process σ. In this section, we will derive this relation assuming that Eq. (7.28) holds. The theorem is, in fact, the simple consequence of the unitary of S-matrix. So, we start with $S^\dagger S = 1$, expand S as $1 + R$ and obtain

$$R + R^\dagger + R^\dagger R = 0\,. \tag{8.1}$$

Then, sandwich it with $\langle \mathbf{p}' |$ and $|\mathbf{p}\rangle$ and insert a completeness relation into the $R^\dagger R$ term to yield

$$\left\langle \mathbf{p}' \right| R \left| \mathbf{p} \right\rangle + \left\langle \mathbf{p} \right| R \left| \mathbf{p}' \right\rangle^* = -\int d^3\mathbf{p}'' \left\langle \mathbf{p}' \right| R^\dagger \left| \mathbf{p}'' \right\rangle \left\langle \mathbf{p}'' \right| R \left| \mathbf{p} \right\rangle\,. \tag{8.2}$$

Next, use the second of Eqs. (7.27) to arrive at

$$\begin{aligned} &\delta\left(E_{\mathbf{p}} - E_{\mathbf{p}'}\right)\left[f\left(\mathbf{p}' \leftarrow \mathbf{p}\right) - f^*\left(\mathbf{p} \leftarrow \mathbf{p}'\right)\right] \\ &\qquad = \frac{i}{2\pi m}\int d^3\mathbf{p}''\,\delta\left(E_{\mathbf{p}'} - E_{\mathbf{p}''}\right)\delta\left(E_{\mathbf{p}''} - E_{\mathbf{p}}\right) f^*\left(\mathbf{p}'' \leftarrow \mathbf{p}'\right) f\left(\mathbf{p}'' \leftarrow \mathbf{p}\right)\,. \end{aligned} \tag{8.3}$$

Using the identity

$$\delta\left(E_{\mathbf{p}'} - E_{\mathbf{p}''}\right)\delta\left(E_{\mathbf{p}''} - E_{\mathbf{p}}\right) = \delta\left(E_{\mathbf{p}} - E_{\mathbf{p}'}\right)\delta\left(E_{\mathbf{p}} - E_{\mathbf{p}''}\right)\,, \tag{8.4}$$

one can simplify this to

$$f\left(\mathbf{p}' \leftarrow \mathbf{p}\right) - f^*\left(\mathbf{p} \leftarrow \mathbf{p}'\right) = \frac{i}{2\pi m}\int d^3\mathbf{p}''\,\delta\left(E_{\mathbf{p}} - E_{\mathbf{p}''}\right) f^*\left(\mathbf{p}'' \leftarrow \mathbf{p}'\right) f\left(\mathbf{p}'' \leftarrow \mathbf{p}\right)\,. \tag{8.5}$$

Now, let us consider the limit of forward scattering $\mathbf{p}' = \mathbf{p}$.[1] By using the property of the delta-function

$$\delta\left[f(x)\right] = \delta(x - x_0)/|f'(x_0)|\,, \tag{8.6}$$

[1] Strictly speaking, the amplitude (and the differential cross section) is not defined in the limit of forward scattering. This is due to the fact that in this limit one cannot distinguish between scattered and unscattered (represented by the first term in Eqs. (7.27)) particles. Normally, however, f is continuous in a however small neighbourhood of the point $\mathbf{p}' = \mathbf{p}$, and one can define it in that point by using this continuity.

the above is written as

$$2i\,\mathrm{Im}\, f(\mathbf{p}\leftarrow\mathbf{p}) = \frac{i}{2\pi m}\int d\Omega\, p''^2 dp'' \frac{m}{p}\delta\left(p-p''\right)\left|f\left(\mathbf{p}''\leftarrow\mathbf{p}\right)\right|^2 , \tag{8.7}$$

(where p denotes $|\mathbf{p}|$) or

$$\mathrm{Im}\, f(\mathbf{p}\leftarrow\mathbf{p}) = \frac{p}{4\pi}\int d\Omega\,|f(\mathbf{p}\leftarrow\mathbf{p})|^2 . \tag{8.8}$$

Substituting $d\sigma/d\Omega$ according to Eq. (7.28), we obtain the desired relation,

$$\mathrm{Im}\, f(\mathbf{p}\to\mathbf{p}) = \frac{p}{4\pi}\sigma(\mathbf{p}) . \tag{8.9}$$

The optical theorem shows that in general the scattering amplitude cannot be purely real and that it has a positive imaginary part near the forward direction. Note also that measurement of the differential cross section in general determines only $|f|$, while by exploiting the optical theorem one can measure $\mathrm{Im}\, f$ and hence $\mathrm{Re}\, f$ separately in the forward direction.

8.2 Cross section and scattering amplitude

The goal of this section is to connect the scattering amplitude f defined in the second of Eqs. (7.27) to the differential cross section, Eq. (7.28). In the quantum scattering problem an incident particle approaches a target in some definite in-state $|\psi_{\mathrm{in}}\rangle$, which we will identify by its momentum-space wavefunction $\psi_{\mathrm{in}}(\mathbf{p}) = \langle\mathbf{p}|\psi_{\mathrm{in}}\rangle$. The corresponding outgoing wavefunction $\psi_{\mathrm{out}}(\mathbf{p}) = \langle\mathbf{p}|\psi_{\mathrm{out}}\rangle$ determines the probability that long after the interaction with the target the particle is found with momentum $\mathbf{p}$. The probability for the particle to emerge with momentum anywhere in the element of solid angle $d\Omega$ about the direction $\mathbf{p}/p$ is obtained by integrating over all p:

$$\omega(d\Omega\leftarrow\psi_{\mathrm{in}}) = d\Omega\int p^2 dp\,|\psi_{\mathrm{out}}(p)|^2 . \tag{8.10}$$

To make reliable measurements of scattering parameters, it is necessary to have multiple scattering events. In classical theory, they are provided by scattering of a steady flow of particles approaching the target with different impact parameters. In quantum theory, we can model this situation as follows. Take some definite state $|\phi_0\rangle$ representing a localized wave packet with zero impact parameter and a momentum distribution peaked around the momentum $\mathbf{p}_0$.[2] To make a "flow", consider states of the form

$$|\phi_{\mathbf{a}}\rangle = e^{-i\mathbf{p}\cdot\mathbf{a}}|\phi_0\rangle , \tag{8.11}$$

that is, $|\phi_{\mathbf{a}}\rangle$ is obtained by rigid displacement of the state $|\phi_0\rangle$ in the lateral direction. The states $|\phi_{\mathbf{a}}\rangle$ represents particles approaching the target with some non-zero impact parameter a.

Having the states $|\phi_{\mathbf{a}}\rangle$ with all a, we can prepare a homogeneous flux of particles moving towards the target as is prescribed by the evolution operator U. As in the classical scattering theory, define the differential cross section $d\sigma/d\Omega$ as

$$N = \frac{d\sigma}{d\Omega}d\Omega , \tag{8.12}$$

where N is the number of particles scattered within the solid angle $d\Omega$ per unit time. We have,

$$\frac{d\sigma}{d\Omega}d\Omega = N = \int d^2a\,\omega(d\Omega\leftarrow\phi_{\mathbf{a}}) . \tag{8.13}$$

[2] We will see below how sharp the momentum distribution should be and why the physical observables like the differential cross section are essentially independent of the precise shape of the state $|\phi_0\rangle$.

Using Eq. (8.10) gives

$$\frac{d\sigma}{d\Omega} = \int d^2a \int dp\, p^2 \left|\psi_{\text{out}}(p)\right|^2 . \tag{8.14}$$

Next, one should express $\psi_{\text{out}}(\mathbf{p})$ through $\psi_{\text{in}}(\mathbf{p}) = \phi_{\mathbf{a}}(\mathbf{p}) = e^{-i\mathbf{p}\cdot\mathbf{a}}\phi_0(\mathbf{p})$:

$$\begin{aligned}\psi_{\text{out}}(\mathbf{p}) &= \int d^3\mathbf{p}' \langle \mathbf{p}|S|\mathbf{p}'\rangle \psi_{\text{in}}(\mathbf{p}') \\ &= \psi_{\text{in}}(\mathbf{p}) + \frac{i}{2\pi m}\int d^3\mathbf{p}'\delta(E_p - E_{p'}) f(\mathbf{p}\leftarrow\mathbf{p}')\psi_{\text{in}}(\mathbf{p}') .\end{aligned} \tag{8.15}$$

We now make the essential restriction that we do not make our observations in the forward direction. Then, the first term in the expression above is excluded and we are left with

$$\psi_{\text{out}}(\mathbf{p}) = \frac{i}{2\pi m}\int d^3\mathbf{p}'\delta\left(E_{\mathbf{p}} - E_{\mathbf{p}'}\right) f\left(\mathbf{p}\leftarrow\mathbf{p}'\right) e^{-i\mathbf{p}'\cdot\mathbf{a}}\phi_0(\mathbf{p}') . \tag{8.16}$$

Substituting this expression to Eq. (8.14) yields

$$\begin{aligned}\frac{d\sigma}{d\Omega} = \frac{1}{(2\pi m)^2}\int d^2a \int p^2 dp \Bigg[\int d^3\mathbf{p}'\delta\left(E_{\mathbf{p}} - E_{\mathbf{p}'}\right) f\left(\mathbf{p}\leftarrow\mathbf{p}'\right) e^{-i\mathbf{p}'\cdot\mathbf{a}}\phi_0(\mathbf{p}') \\ \times \int d^3\mathbf{p}''\delta\left(E_{\mathbf{p}} - E_{\mathbf{p}''}\right) f^*\left(\mathbf{p}\leftarrow\mathbf{p}''\right) e^{i\mathbf{p}''\cdot\mathbf{a}}\phi_0^*(\mathbf{p}'')\Bigg] .\end{aligned} \tag{8.17}$$

The first integral to evaluate is the one over a:

$$\int d^2a\, e^{-i\mathbf{a}\cdot\mathbf{p}'+i\mathbf{a}\cdot\mathbf{p}''} = (2\pi)^2\delta^{(2)}\left(p'_\perp - p''_\perp\right) . \tag{8.18}$$

Since the a-integral is evaluated over a plane orthogonal to the direction of the beam, the delta-function it results in constrain only the orthogonal part of the momentum, hence the subscript $_\perp$. This delta-function can be combined with the other two delta-functions in Eq. (8.17) as follows,

$$\begin{aligned}&\delta\left(E_{\mathbf{p}} - E_{\mathbf{p}'}\right)\delta\left(E_{\mathbf{p}} - E_{\mathbf{p}''}\right)\delta^{(2)}\left(p'_\perp - p''_\perp\right) \\ &\qquad = \delta\left(E_{\mathbf{p}} - E_{\mathbf{p}'}\right)\delta\left(\frac{p'^2_\parallel}{2m} - \frac{p''^2_\parallel}{2m}\right)\delta^{(2)}\left(p'_\perp - p''_\perp\right) \\ &\qquad = \delta\left(E_{\mathbf{p}} - E_{\mathbf{p}'}\right)\frac{m}{|p_\parallel|}\delta\left(p'_\parallel - p''_\parallel\right)\delta^{(2)}\left(p'_\perp - p''_\perp\right) \\ &\qquad = \delta\left(E_{\mathbf{p}} - E_{\mathbf{p}'}\right)\frac{m}{|p_\parallel|}\delta^{(3)}\left(\mathbf{p}' - \mathbf{p}''\right) .\end{aligned} \tag{8.19}$$

In the first equality, we used the constraint from $\delta^{(2)}\left(p'_\perp - p''_\perp\right)$ to simplify $\delta\left(E_{\mathbf{p}} - E_{\mathbf{p}''}\right)$ and in the second equality we used the property of dirac delta function $\delta[f(x)] = \delta(x-x_0)/|f'(x_0)|$. Now, Eq. (8.17) becomes

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \frac{1}{m^2}\int p^2 dp \int d^3\mathbf{p}' d^3\mathbf{p}''\delta\left(E_{\mathbf{p}} - E_{\mathbf{p}'}\right)\phi(\mathbf{p}')\phi^*(\mathbf{p}'') f\left(\mathbf{p}\leftarrow\mathbf{p}'\right) f^*\left(\mathbf{p}\leftarrow\mathbf{p}''\right)\frac{m}{|p_\parallel|}\delta^{(3)}\left(\mathbf{p}' - \mathbf{p}''\right) \\ &= \frac{1}{m}\int p^2 dp \int \frac{d^3\mathbf{p}'}{|p_\parallel|}\frac{m}{p}\delta\left(p - p'\right)\left|\phi(\mathbf{p}')\right|^2\left|f\left(\mathbf{p}\leftarrow\mathbf{p}'\right)\right|^2 \\ &= \int d^3\mathbf{p}'\frac{p'}{p'_\parallel}\left|\phi(\mathbf{p}')\right|^2\left|f\left(\mathbf{p}\leftarrow\mathbf{p}'\right)\right|^2 .\end{aligned}$$

(8.20)

It remains to do the final and crucial step. Remember that $\phi(\mathbf{p}')$ is peaked around $\mathbf{p}_0$. So, if the region where $\phi(\mathbf{p}')$ is appreciably different from zero is so small that the variation of the amplitude $f(\mathbf{p} \leftarrow \mathbf{p}')$ in this region is insignificant, then one can replace $f(\mathbf{p} \leftarrow \mathbf{p}')$ and $p'/p'_{\|}$ by their values at $\mathbf{p} = \mathbf{p}_0$. This gives,

$$\frac{d\sigma}{d\Omega} = |f(\mathbf{p} \leftarrow \mathbf{p}_0)|^2 \,, \tag{8.21}$$

because the one remaining integral is just the normalisation integral of the wavefunction ϕ. It is important to note that the result (8.21) is independent of the precise shape of ϕ, provided only that $\phi(\mathbf{p})$ is sufficiently peaked around $\mathbf{p}_0$. Having established the relation between the physically observed quantity $d\sigma/d\Omega$ and the scattering amplitude, we should now proceed to developing the formalism for computing the latter.

8.3 Green's function and Møller operators

The definitions of Møller operators (7.6), (7.7) involve the product $U^\dagger(t)U_0(t)$. It will prove useful to represent it as

$$\begin{aligned} U^\dagger(t)U_0(t) &= 1 + \int_0^t dt' \frac{d}{dt'} \left[U^\dagger(t')U_0(t')\right] \\ &= 1 + \int_0^t dt' \frac{d}{dt'} \left[e^{iHt'} e^{-iH_0 t'}\right] \\ &= 1 + \int_0^t dt' i e^{iHt'} (H - H_0) e^{-iH_0 t'} \\ &= 1 + i \int_0^t dt' U^\dagger(t') V U_0(t') \,. \end{aligned} \tag{8.22}$$

Plugging the above expression into Eq. (7.6), we get

$$\begin{aligned} |\psi_0\rangle &= |\psi_{\text{out}}\rangle + i \int_0^\infty d\tau U^\dagger(\tau) V U_0(\tau) |\psi_{\text{out}}\rangle \\ &= |\psi_{\text{out}}\rangle + i \lim_{\varepsilon \to 0} \int_0^\infty d\tau e^{-\varepsilon\tau} U^\dagger(\tau) V U_0(\tau) |\psi_{\text{out}}\rangle \\ &= |\psi_{\text{out}}\rangle + i \lim_{\varepsilon \to 0} \int d^3\mathbf{p} \int_0^\infty d\tau e^{-\varepsilon\tau + iH\tau} V e^{-iE_p\tau} |\mathbf{p}\rangle \langle \mathbf{p} | \psi_{\text{out}}\rangle \\ &= |\psi_{\text{out}}\rangle + \lim_{\varepsilon \to 0} \int d^3\mathbf{p} \frac{1}{E_p - H - i\varepsilon} V |\mathbf{p}\rangle \langle \mathbf{p} | \psi_{\text{out}}\rangle \,. \end{aligned} \tag{8.23}$$

From the first to second line, we introduced a regulator $\lim_{\varepsilon \to 0} e^{-\varepsilon\tau}$ to ensure the convergence of the integral; from the second to third line we inserted a completeness relation and write out the evolution operators explicitly; in the final step we performed the integral by treating H formally as a c-number. In the last line, an object of the form

$$G(z) = \frac{1}{z - H} \,, \tag{8.24}$$

where z is a complex number, makes its appearance. It is called the Green's operator (or the Green's function, see Addendum A for the motivation of this name). In terms of the Green's function, we can write (8.23) as

$$|\psi_0\rangle = |\psi_{\text{out}}\rangle + i \lim_{\varepsilon \to 0} \int d^3\mathbf{p}\, G(E_p - i\varepsilon) V |\mathbf{p}\rangle \langle \mathbf{p} | \psi_{\text{out}}\rangle \,. \tag{8.25}$$

If one repeats the above analysis with $|\psi_{\rm in}\rangle$ instead of $|\psi_{\rm out}\rangle$, one obtains

$$|\psi_0\rangle = |\psi_{\rm in}\rangle + \lim_{\varepsilon\to 0}\int d^3\mathbf{p}\, G(E_p + i\varepsilon)\, V\,|\mathbf{p}\rangle\,\langle\mathbf{p}\,|\psi_{\rm in}\rangle\ . \tag{8.26}$$

Comparing them with Eqs. (7.6), (7.7), we find

$$\Omega_\pm = 1 + \lim_{\varepsilon\to 0}\int d^3\mathbf{p} G(E_p \pm i\varepsilon) V\,|\mathbf{p}\rangle\,\langle\mathbf{p}|\ . \tag{8.27}$$

This is an important form of the Møller operators, since it represents explicitly the interaction associated with V.

Addendum A To understand the name "Green's operator", assume that the operator $(z-H)^{-1}$ does actually exist and is defined everywhere in the Hilbert space $\mathscr{H}$ (later we will see that this is true for any z with $\mathrm{Im}\, z \neq 0$). In this case it is clear from the definition that, for example,

$$(z-H_0)G_0(z) = 1\ , \quad G_0(z) = \frac{1}{z-H_0}\ . \tag{8.28}$$

In the x-representation, this means that

$$\langle x|\, z - H_0\,|x'\rangle = \delta(x-x')\ , \tag{8.29}$$

or, inserting the completeness relation,

$$\begin{aligned}
&\int dx''\,\langle x|\,(z-H_0)\,|x''\rangle\,\langle x''|\,G_0\,|x'\rangle \\
&= \int dx''\left[z\delta(x-x'') + \frac{\nabla^2}{2m}\delta(x-x'')\right]\langle x''|\,G_0\,|x'\rangle \\
&= \left(z + \frac{\nabla^2}{2m}\right)\langle x|\,G_0\,|x'\rangle = \delta(x-x')\ .
\end{aligned} \tag{8.30}$$

Thus, the coordinate-space matrix element of the free Green's operator $G_0(z)$ is the Green's function for the differential operator $z+\nabla^2/2m$. In exactly the same way the matrix element of $G(z)$ is the Green's function for the operator $z+\nabla^2/2m-V$.

▪ Exercise 8.1 — On integrals involving a delta-function.

1. Compute the integral

$$\int_{-\infty}^{\infty} dx\, f(x)\delta(ax^2+bx+c) \tag{8.31}$$

with $f(x)$ the real function and a, b, c the reals.

2. Compute the radial part of the integral

$$\int d^3\mathbf{p}\, f(\mathbf{p})\delta(E_{p'} - E_p) \tag{8.32}$$

with f the real function of the momentum $\mathbf{p}$.

▪

▪ Exercise 8.2 — Free particle's Green function in three dimensions.

Recall that the Green function for the free Hamiltonian $\hat{H}_0$ is written as

$$\hat{G}_0(z) = \frac{1}{z-\hat{H}_0},\ \ z = x + i\varepsilon\,. \tag{8.33}$$

1. Show that

$$\langle \mathbf{x}|\hat{G}_0(z)|\mathbf{x}'\rangle = \frac{1}{(2\pi)^3}\int d^3\mathbf{p}\frac{e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')}}{z-E_p}\,, \quad E_p = \frac{p^2}{2m}\,, \tag{8.34}$$

   where we put $\hbar = 1$.
2. Compute the integral above to yield

$$\langle \mathbf{x}|\hat{G}_0(z)|\mathbf{x}'\rangle = -\frac{m}{2\pi}\frac{e^{i\sqrt{2mz}\,|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}\,. \tag{8.35}$$

   Hint: First, compute the angular part of the integral. After that, close the contour of integration and use the method of residues. Note that the prescription $z = x + i\varepsilon$, $\varepsilon > 0$ plays a crucial role in this calculation.
3. Check that the result (8.35) is indeed the Green function of the stationary Schrodinger equation, that is

$$\langle \mathbf{x}|(z-\hat{H}_0)\hat{G}_0(z)|\mathbf{x}'\rangle = \delta^{(3)}(\mathbf{x}-\mathbf{x}')\,. \tag{8.36}$$

4. Calculate the difference

$$\langle \mathbf{x}|\hat{G}_0(E+i\varepsilon) - \hat{G}_0(E-i\varepsilon)|\mathbf{x}'\rangle \tag{8.37}$$

   between the values of $\hat{G}_0(z)$ on the upper and the lower sides of the branch cut at $E > 0$.
5. Find an asymptotic behavior of the Green function $\langle \mathbf{x}|\hat{G}_0(z)|\mathbf{x}'\rangle$ in the limit of large separation of points (say, send $|\mathbf{x}| \to \infty$ while keeping $|\mathbf{x}'|$ finite).

▪

▪ **Exercise 8.3 — Friedel sum rule.** Let $N(E) = \sum_n \delta(E - E_n)$ be the density of eigenstates of the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$, and $N_0(E)$ the density for the free Hamiltonian $\hat{H}_0$.

1. Express $N(E)$ through the Green function $\hat{G}$ of $\hat{H}$.
   Hint: Use the relation

$$\frac{1}{x+i\varepsilon} = -i\pi\delta(x) + \mathscr{P}\frac{1}{x}\,, \tag{8.38}$$

   where $\mathscr{P}$ denotes the principal value.
2. Deduce the following sum rule,

$$N(E) - N_0(E) = \frac{1}{\pi}\frac{d}{dE}\arg\det\left(\hat{G}(E+i\varepsilon)\hat{G}_0^{-1}(E+i\varepsilon)\right)\,, \tag{8.39}$$

   where $\hat{G}_0$ is the Green function of the free Hamiltonian.

▪

▪ **Exercise 8.4 — Slow scattering in a gas.** Consider a non-relativistic particle of momentum p, scattering off the potential with a characteristic range R. We say that the particle is slow if

$$p \lesssim \frac{\hbar}{R}\,. \tag{8.40}$$

Considering this regime is important because, as we will see later, the scattering amplitudes can behave qualitatively different depending on whether the condition (8.40) fulfills or not.

1. The range of the potential between two hydrogen atoms is approximately 4. For a gas in thermal equilibrium, find a numerical estimate of the temperature below which the atom-atom scattering is essentially slow.

▪

Lecture 9

> Analytic structure of Green's function; Lippmann-Schwinger equation; S-matrix via Green's function; S-matrix in terms of T-matrix; perturbation theory for scattering amplitude; Born approximation.

9.1 Analytic structure of Green's function, Lippman-Schwinger equation and T-matrix

As was discussed before, the spectrum of the full Hamiltonian H, in general, consists of a discrete set of negative eigenvalues corresponding to bound states $|n\rangle$, $n = 1, ..., N$, followed by a continuous set of positive eigenvalues corresponding to scattering states $|\mathbf{q}\rangle = \Omega_+ |\mathbf{p}\rangle$. Recall that, according to Eq. (7.18), $|\mathbf{q}\rangle$ is indeed an eigenstate of H with the eigenvalue $E_q = E_p = p^2/2m$. The completeness of eigenstates of H allows us to use them to resolve identity:

$$1 = \sum_{n=1}^{N} |n\rangle \langle n| + \int d^3\mathbf{q} \, |\mathbf{q}\rangle \langle \mathbf{q}| \ . \tag{9.1}$$

Applying the Green's operator $G(z)$ to the both sides of this equality yields

$$G(z) = \sum_{n=1}^{N} \frac{|n\rangle \langle n|}{z - E_n} + \int d^3\mathbf{q} \frac{|\mathbf{q}\rangle \langle \mathbf{q}|}{z - E_q} \ . \tag{9.2}$$

This representation of the Green's operator allows us to capture its analytic properties as a function of the complex variable z. First of all, we see that for any z not equal neither to a negative eigenvalue nor to a positive real number, the operator (9.2) is well defined on any state from the Hilbert space $\mathscr{H}$. We say that the Green's operator is analytic for those z, meaning that for any two states $|\psi\rangle$, $|\phi\rangle$ from $\mathscr{H}$ the function $\langle \psi | G(z) | \phi \rangle$ is analytic. In the same sense, $G(z)$ has poles at $z_n = E_n$ corresponding to bound states, and a branch cut along the line of real positive z (since E_q ranges from 0 to ∞), corresponding to scattering states. From Eq. (9.2) we see that the residue of $G(z)$ at some $z_n = E_n$ is the projection operator onto the corresponding bound state,

$$\mathrm{res}_{z=E_n} G(z) = |n\rangle\langle n| \ . \tag{9.3}$$

The Green's operator $G_0(z)$ corresponding to the free Hamiltonian H_0 possesses no poles but only the branch cut along the real positive line.

The above consideration leads us to the conclusion that knowledge of the analytic structure of the Green's operator $G(z)$ of a Hamiltonian H for all z is equivalent to knowledge of a complete

solution of the corresponding eigenvalue problem, and that $G(z)$ is analytic except on the spectrum of H. It should come as no surprise then that finding $G(z)$ is precisely as hard as solving the eigenvalue problem. For this reason it is useful to have an equation that relates $G(z)$ to some known operator. The natural choice for the latter is the free particle Green's operator, $G_0(z)$. The equation relating $G(z)$ and $G_0(z)$ is called the resolvent equation or Lippmann-Schwinger equation for $G(z)$. To get it, we use the obvious operator identity

$$A^{-1} = B^{-1} + B^{-1}(B-A)A^{-1} \,. \tag{9.4}$$

Setting $A = z - H$ and $B = z - H_0$ gives one form of the Lippmann-Schwinger equation

$$G(z) = G_0(z) + G_0(z)VG(z) \,. \tag{9.5}$$

Alternatively, if we choose $A = z - H_0$ and $B = z - H$, we obtain

$$G_0(z) = G(z) + G(z)(-V)G_0(z) \tag{9.6}$$

or, equivalently,

$$G(z) = G_0(z) + G(z)VG_0(z) \,, \tag{9.7}$$

which is another form of the Lippmann-Schwinger equation. As we will see, these two equations are one of the foundation stones of the time-independent scattering theory.

Let us now introduce another operator $T(z)$, or "T-matrix". It is defined in terms of the Green's operator $G(z)$ as

$$T(z) = V + VG(z)V \,. \tag{9.8}$$

As a function of z, the operator $T(z)$ exhibits the same analytic properties as $G(z)$. Using the T-matrix, one can obtain more useful relations between $G(z)$ and $G_0(z)$. Applying $G_0(z)$ to the above equation from the left, we have

$$G_0(z)T(z) = G_0(z)V + G_0(z)VG(z)V = (G_0(z) + G_0(z)VG(z))V = G(z)V \,, \tag{9.9}$$

where in the last step Eq. (9.5) was used. If we instead add $G_0(z)$ from the right, we get

$$T(z)G_0(z) = VG_0(z) + VG(z)VG_0(z) = V\,(G_0(z) + G(z)VG_0(z)) = VG(z) \,, \tag{9.10}$$

where Eq. (9.7) in the last step.

Let us mention two more identities involving the T-matrix and the Green's operators $G(z)$ and $G_0(z)$. Applying Eq. (9.9) to Eq. (9.7), one obtains

$$G(z) = G_0(z) + G_0(z)T(z)G_0(z) \,. \tag{9.11}$$

Finally, applying Eq. (9.9) to (9.8) yields

$$T(z) = V + VG_0(z)T(z) \,. \tag{9.12}$$

The last equation is known as the Lippmann-Schwinger equation for $T(z)$ and is the starting point of many methods for calculating the T-matrix.

9.2 S-matrix via Green's function and T-matrix

In the limiting formula for the S-matrix (7.15), let us take $t' = -t$ to obtain

$$S = \lim_{t\to\infty} e^{iH_0 t} e^{-2iHt} e^{iH_0 t} \,. \tag{9.13}$$

Differentiating the expression in the r.h.s. with respect to t gives

$$\frac{d}{dt}\left[e^{iH_0 t} e^{-2iHt} e^{iH_0 t}\right] = -i\left[e^{iH_0 t} V e^{-2iHt} e^{iH_0 t} + e^{iH_0 t} e^{-2iHt} V e^{iH_0 t}\right] \,. \tag{9.14}$$

Integrating this over t from 0 to ∞ restores the original expression, and we have

$$S = 1 - i \lim_{\varepsilon\to+0} \int_0^\infty dt\, e^{-\varepsilon t}\left[e^{iH_0 t} V e^{-2iHt} e^{iH_0 t} + e^{iH_0 t} e^{-2iHt} V e^{iH_0 t}\right] \,, \tag{9.15}$$

where the regulator $e^{-\varepsilon t}$ was introduced to ensure the convergence of the integral. The S-matrix element is now given by

$$\begin{aligned}\langle \mathbf{p}'|S|\mathbf{p}\rangle &= \delta^{(3)}(\mathbf{p}-\mathbf{p}') - i \lim_{\varepsilon\to+0} \int_0^\infty dt\, \langle \mathbf{p}'|V e^{-\varepsilon t + iE_{p'}t + iE_p t - 2iHt} + e^{-\varepsilon t + iE_{p'}t + iE_p t - 2iHt} V|\mathbf{p}\rangle \\ &= \delta^{(3)}(\mathbf{p}-\mathbf{p}') + \frac{1}{2}\lim_{\varepsilon\to+0} \langle \mathbf{p}'|VG\left(\frac{E_{\mathbf{p}'}+E_{\mathbf{p}}}{2}+i\varepsilon\right) + G\left(\frac{E_{\mathbf{p}'}+E_{\mathbf{p}}}{2}+i\varepsilon\right)V|\mathbf{p}\rangle \,.\end{aligned} \tag{9.16}$$

Using the relations of section 9.1 involving the operators G, G_0, V and T, the above can also be written as

$$\begin{aligned}\left\langle \mathbf{p}'\right| S \left|\mathbf{p}\right\rangle &= \delta^{(3)}\left(\mathbf{p}'-\mathbf{p}\right) - \frac{1}{2}\lim_{\varepsilon\to+0}\left\langle \mathbf{p}'\right| VG+GV \left|\mathbf{p}\right\rangle \\ &= \delta^{(3)}\left(\mathbf{p}'-\mathbf{p}\right) - \frac{1}{2}\lim_{\varepsilon\to+0}\left\langle \mathbf{p}'\right| TG_0+G_0T \left|\mathbf{p}\right\rangle \\ &= \delta^{(3)}\left(\mathbf{p}'-\mathbf{p}\right) - \frac{1}{2}\lim_{\varepsilon\to+0}\left\langle \mathbf{p}'\right| T\left(\frac{E_{\mathbf{p}'}+E_{\mathbf{p}}}{2}+i\varepsilon\right) \left|\mathbf{p}\right\rangle \left[\frac{1}{\frac{E_{\mathbf{p}'}+E_{\mathbf{p}}}{2}+i\varepsilon-E_{\mathbf{p}}} + \frac{1}{\frac{E_{\mathbf{p}'}+E_{\mathbf{p}}}{2}+i\varepsilon-E_{\mathbf{p}'}}\right] \\ &= \delta^{(3)}\left(\mathbf{p}'-\mathbf{p}\right) - \frac{1}{2}\lim_{\varepsilon\to+0}\left\langle \mathbf{p}'\right| T\left(\frac{E_{\mathbf{p}'}+E_{\mathbf{p}}}{2}+i\varepsilon\right) \left|\mathbf{p}\right\rangle \left[\frac{2}{E_{\mathbf{p}'}-E_{\mathbf{p}}+i\varepsilon} + \frac{2}{E_{\mathbf{p}}-E_{\mathbf{p}'}+i\varepsilon}\right] \,.\end{aligned} \tag{9.17}$$

From the first to second line we used Eqs. (9.9) and (9.10); from the second to third line we simply acted by G_0 on one of the momentum eigenstates; the last step is just a simple algebra. Now, one can use the relation

$$\frac{1}{x+i\varepsilon} = \mathscr{P}\left(\frac{1}{x}\right) - i\pi\delta(x) \,, \tag{9.18}$$

where $\mathscr{P}[f(x)]$ stands for the principal value of the function $f(x)$ (see Addendum A for the reminder of the proof of Eq. (9.18)). This gives the relation between the S-matrix and T-matrix:

$$\left\langle \mathbf{p}'\right| S \left|\mathbf{p}\right\rangle = \delta^{(3)}\left(\mathbf{p}'-\mathbf{p}\right) - 2\pi i\delta\left(E_{\mathbf{p}}-E_{\mathbf{p}'}\right)\left\langle \mathbf{p}\right| T\left(E_{\mathbf{p}}+i\varepsilon\right)\left|\mathbf{p}'\right\rangle \,. \tag{9.19}$$

Recall that in lecture 9 we introduced the t-function, Eqs. (7.27). We now see that

$$t(\mathbf{p}'\leftarrow\mathbf{p}) = \langle \mathbf{p}'|T(E_p+i\varepsilon)|\mathbf{p}\rangle = -\frac{1}{(2\pi)^2 m} f(\mathbf{p}'\leftarrow\mathbf{p}) \,, \quad \text{if } E_{p'} = E_p \,. \tag{9.20}$$

Let us make an important comment concerning the T-matrix and its matrix elements. Because of the factor $\delta(E_{p'} - E_p)$ in Eqs. (7.27), the quantity $t(\mathbf{p}' \leftarrow \mathbf{p})$ is defined only for $E_{p'} = E_p$. That is, in the space of variables $\mathbf{p}'$ and $\mathbf{p}$ the function $t(\mathbf{p}' \leftarrow \mathbf{p})$ is defined only on the "energy shell" $p'^2 = p^2$. So, if the T-matrix is defined according to Eqs. (7.27) and (9.19), it is said to be *on-shell*. As far as the observation of scattering experiments is concerned, only the on-shell T-matrix is relevant, since its knowledge is enough to determine the S-matrix. In calculations, however, it is useful to define the T-matrix according to Eq. (9.8), in which case it is, in general, an *off-shell* operator. $T(z)$ becomes on-shell for the particular values $z = E_p + i\varepsilon$, $\varepsilon \to +0$, and for $E_{p'} = E_p$.

9.3 Perturbation theory for scattering amplitude

In general, the S-matrix cannot be found in a closed form. One, therefore, has to appeal to approximation methods. One of them is the perturbation theory based on the Born series. For this to work, assume that the interaction term in the full Hamiltonian H is "small" in the sense that one can write

$$H = H_0 + \lambda V \tag{9.21}$$

with $\lambda \ll 1$. Next, write the Lippman-Schwinger equation for T-matrix (9.12) in the form

$$T = (1 - \lambda V G_0)^{-1} \lambda V \ . \tag{9.22}$$

Assume that the inverse can be expanded as a binomial series

$$(1 - \lambda V G_0)^{-1} = 1 + \lambda V G_0 + \lambda^2 V G_0 V G_0 + ... \tag{9.23}$$

Then, for the T-matrix we have the series

$$T = \lambda V + \lambda^2 V G_0 V + \lambda^3 V G_0 V G_0 V + ... \tag{9.24}$$

This is called the Born series. Its convergence can be ensured provided that λ is small enough and that the potential V satisfies the conditions listed in section 7.2 (see section 9-a of [7] for the proof). Moreover, normally the first several terms in the series approximate the result with the accuracy sufficient for practical purposes. If we cut the series just after the first term, we obtain the first Born approximation,

$$T^{(1)} = \lambda V \ . \tag{9.25}$$

Taking into account the λ^2-term leads to the second Born approximation,

$$T^{(1)} + T^{(2)} = \lambda V + \lambda^2 V G_0 V \ , \tag{9.26}$$

and so on. For the function $t(\mathbf{p}' \leftarrow \mathbf{p})$ and the scattering amplitude $f(\mathbf{p}' \leftarrow \mathbf{p})$ the first Born approximation implies (we absorb λ into V for convenience)

$$t^{(1)}(\mathbf{p}' \leftarrow \mathbf{p}) = \langle \mathbf{p}' | V | \mathbf{p} \rangle \tag{9.27}$$

and

$$\begin{aligned} f^{(1)}(\mathbf{p}' \leftarrow \mathbf{p}) &= -(2\pi)^2 m \left\langle \mathbf{p}' | V | \mathbf{p} \right\rangle \\ &= -(2\pi)^2 m \int d^3\mathbf{x} \left\langle \mathbf{p}' | V \, | \mathbf{x} \right\rangle \left\langle \mathbf{x} | \, \mathbf{p} \right\rangle \\ &= -\frac{m}{2\pi} \int d^3\mathbf{x} \, e^{-i\mathbf{q}\cdot\mathbf{x}} V(\mathbf{x}) \ , \end{aligned} \tag{9.28}$$

where the vector $\mathbf{q} = \mathbf{p}' - \mathbf{p}$ is called the momentum transfer.

The first Born approximation for the scattering amplitude (9.28) is one of the most important formulas in scattering theory. Note that it depends on the momenta $\mathbf{p}$ and $\mathbf{p}'$ only through their difference $\mathbf{q}$. In fact, up to a numerical factor, $f^{(1)}(\mathbf{p}' \leftarrow \mathbf{p})$ is simply the Fourier transform of the potential, evaluated at $\mathbf{q}$.

The next order terms in the expansion of the T-matrix can be calculated a similar way. For example,

$$\begin{aligned} \langle \mathbf{p}' | T^{(2)} | \mathbf{p} \rangle &= \langle \mathbf{p}' | V G_0 V | \mathbf{p} \rangle \\ &= \int d^3\mathbf{p}'' \langle \mathbf{p}' | V | \mathbf{p}'' \rangle \langle \mathbf{p}'' | G_0 V | \mathbf{p} \rangle \\ &= \int d^3\mathbf{p}'' \langle \mathbf{p}' | V | \mathbf{p}'' \rangle \frac{1}{\frac{E_{\mathbf{p}'} - E_{\mathbf{p}}}{2} + i\varepsilon - E_{\mathbf{p}''}} \langle \mathbf{p}'' | V | \mathbf{p} \rangle \ . \end{aligned} \tag{9.29}$$

The matrix elements $\langle \mathbf{p}' | V | \mathbf{p}'' \rangle$ and $\langle \mathbf{p}'' | V | \mathbf{p} \rangle$ have already been evaluated in Eq. (9.28); they are the Fourier transforms of $V(\mathbf{x})$ at $\mathbf{p}' - \mathbf{p}''$ and $\mathbf{p}'' - \mathbf{p}$ correspondingly.

As an application of the first Born approximation, let us compute the differential cross section of the Yukawa potential

$$V(r) = \frac{\alpha}{r} e^{-\mu r} \ . \tag{9.30}$$

This potential satisfies the requirements of section 7.2; in the limit $\mu \to 0$ it reduces to the Coulomb potential. From Eq. (9.28) we have

$$f^{(1)}(\mathbf{p}' \leftarrow \mathbf{p}) = -\frac{m}{2\pi} \int d^3\mathbf{x}\, e^{-i\mathbf{q}\cdot\mathbf{x}} \frac{\alpha}{|\mathbf{x}|} e^{-\mu|\mathbf{x}|} \ . \tag{9.31}$$

In spherical coordinates this becomes

$$\begin{aligned} f^{(1)}(\mathbf{p}' \leftarrow \mathbf{p}) &= -\frac{m}{2\pi} \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \int_0^{\infty} r^2 dr e^{-iqr\cos\theta} \frac{\alpha}{r} e^{-\mu r} \\ &= -\frac{2m\alpha}{|\mathbf{q}|^2 + \mu^2} \ . \end{aligned} \tag{9.32}$$

The magnitude of the momentum transfer is given by

$$|\mathbf{q}|^2 = |\mathbf{p} - \mathbf{p}'|^2 = |\mathbf{p}|^2 + |\mathbf{p}'|^2 - 2|\mathbf{p}||\mathbf{p}'|\cos\theta = 4p^2 \sin^2\frac{\theta}{2} \ , \tag{9.33}$$

where θ is the angle between $\mathbf{p}$ and $\mathbf{p}'$. Thus,

$$\frac{d\sigma}{d\Omega} \approx |f^{(1)}|^2 = \frac{(2m\alpha)^2}{\left(\mu^2 + 4p^2 \sin^2\frac{\theta}{2}\right)^2} \ . \tag{9.34}$$

For the discussion of the accuracy of the first Born approximation in this case see Exercise 9.9. Note that in the limit $\mu \to 0$ the above expression coincides with the Rutherford cross section; for more on this, see Exercise 9.8).

Addendum A It is useful to remind here some basic facts from the theory of generalized functions (or distributions), since they are used intensively in quantum physics.[1]

[1] For a detailed exposition of this theory see, e.g., [8].

As a first step, one defines the vector space of *test* functions. The latter is usually taken to be the set $\mathscr{D}(\mathbb{R})$ of infinitely differentiable functions with a compact support in $\mathbb{R}$ (for simplicity, we consider the one-dimensional case and will write simply $\mathscr{D}$). A basic example of such function is the Gaussian "hat":

$$\omega_a(x) = \begin{cases} Ce^{-\frac{a^2}{a^2-|x|^2}}, & |x| \leqslant a \\ 0, & |x| > a \end{cases} \tag{9.35}$$

with some normalization constant C. Other functions from $\mathscr{D}$ are obtained by taking linear combinations of $\omega_a(x)$. The set $\mathscr{D}$ is quite rich and, in fact, is dense in $\mathscr{L}_2(\mathbb{R})$.

Define now the vector space $\mathscr{D}'(\mathbb{R})$ (we will write simply $\mathscr{D}'$) of *generalized* functions or *distributions* as a space of all linear continuous functionals on $\mathscr{D}$. A functional f maps a function $\varphi \in \mathscr{D}$ to a real number; denote the result of this mapping as (f,φ). Some examples of the functionals from $\mathscr{D}'$ are straightforward. With any integrable (on $\mathbb{R}$) function f one can associate the functional (let us call it also f) such that for any $\varphi \in \mathscr{D}$

$$(f,\varphi) = \int f(x)\varphi(x)dx\,. \tag{9.36}$$

The functionals of this kind are called *regular*. Not all elements of $\mathscr{D}'$ are regular functionals. The most famous example of a *singular* functional is the Dirac delta-function δ. Its action on $\mathscr{D}$ is defined as

$$(\delta,\varphi) = \varphi(0)\,. \tag{9.37}$$

It is easy to prove that no integrable function can be associated with the delta-function.

Consider the functional $\mathscr{P}\frac{1}{x}$ called the *principal value* of the integral of $1/x$. Its action on $\mathscr{D}$ is defined as

$$(\mathscr{P}\frac{1}{x},\varphi) \equiv \mathrm{Vp}\int \frac{\varphi(x)}{x}dx = \lim_{\varepsilon\to+0}\left(\int_{-\infty}^{-\varepsilon} + \int_{\varepsilon}^{\infty}\right)\frac{\varphi(x)}{x}dx\,. \tag{9.38}$$

Let us now prove the Sokhotski formula:

$$\lim_{\varepsilon\to+0}\int \frac{\varphi(x)}{x+i\varepsilon}dx = -i\pi\varphi(0) + \mathrm{Vp}\int\frac{\varphi(x)}{x}dx \tag{9.39}$$

for any $\varphi \in \mathscr{D}$. Since $\varphi(x)$ has a final support, there exists R such that $\varphi(x) = 0$ for $|x| > R$. Then,

$$\begin{aligned}\lim_{\varepsilon\to+0}\int \frac{\varphi(x)}{x+i\varepsilon}dx &= \lim_{\varepsilon\to+0}\int_{-R}^{R}\frac{x-i\varepsilon}{x^2+\varepsilon^2}\varphi(x)dx \\ &= \varphi(0)\lim_{\varepsilon\to+0}\int_{-R}^{R}\frac{x-i\varepsilon}{x^2+\varepsilon^2}dx + \lim_{\varepsilon\to+0}\int_{-R}^{R}\frac{x-i\varepsilon}{x^2+\varepsilon^2}(\varphi(x)-\varphi(0))dx \\ &= -2i\varphi(0)\lim_{\varepsilon\to+0}\arctan\frac{R}{\varepsilon} + \int_{-R}^{R}\frac{\varphi(x)-\varphi(0)}{x}dx \\ &= -i\pi\varphi(0) + \mathrm{Vp}\int\frac{\varphi(x)}{x}dx\end{aligned} \tag{9.40}$$

(the last step is a little exercise). Thus, in terms of distributions

$$\frac{1}{x+i\varepsilon} = -i\pi\delta(x) + \mathscr{P}\frac{1}{x}\,,\quad \varepsilon\to+0\,. \tag{9.41}$$

Similarly,

$$\frac{1}{x-i\varepsilon} = i\pi\delta(x) + \mathscr{P}\frac{1}{x}\,,\quad \varepsilon\to+0\,. \tag{9.42}$$

▪ **Exercise 9.1 — Cauchy's theorem and the completeness relation.** Let $G(z) = \dfrac{1}{z-H}$, where H is a Hamiltonian containing a finite amount of bound states $|n\rangle$ with energies $E_n < 0$ and a continuous spectrum $|p\rangle$ beginning at $E = 0$.

1. Using the completeness relation for the eigenstates of H,

$$\sum_n |n\rangle\langle n| + \int dp|p\rangle\langle p| = 1 \,, \tag{9.43}$$

prove that

$$\oint_C G(z)dz = 2\pi i \sum_n |n\rangle\langle n| \,, \tag{9.44}$$

where the contour C is shown in figure 9.1.

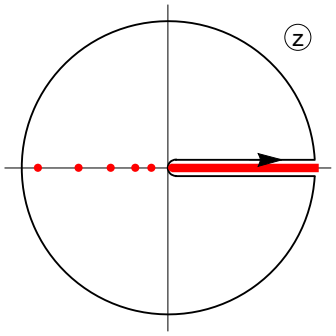


Figure 9.1: The contour of integration C. Red dots mark the bound states of H, the red line represents the branch cut corresponding to the continuous spectrum.

▪

▪ **Exercise 9.2 — Optical theorem in the Born approximation.** Recall that the optical theorem is an *exact* relation between the scattering amplitude in the forward direction $f(\mathbf{p} \leftarrow \mathbf{p})$ and the total cross section of the scattering process,

$$\sigma = \frac{4\pi}{p} \mathrm{Im}\, f(\mathbf{p} \leftarrow \mathbf{p}) \,. \tag{9.45}$$

Suppose that the Hamiltonian H of the scattering system is of the form that permits the usage of the Born approximation. In particular, $H = H_0 + \lambda V$ with H_0 the free Hamiltonian and λ the small parameter. Then, the both sides of Eq. (9.45) can be written as series with respect to λ, and the terms with the same power of λ must coincide.

1. Check explicitly the relation (9.45) to the first nontrivial order in λ.

▪

▪ **Exercise 9.3 — Scattering amplitude in a spherically-symmetric potential.** Consider the non-relativistic particle of mass m and momentum p moving in a spherically-symmetric potential $V(r)$.

1. Show that in the first Born approximation the scattering amplitude is written as

$$f(\mathbf{p}' \leftarrow \mathbf{p}) = -\frac{2m}{q} \int_0^\infty rV(r)\sin(qr)dr \,, \tag{9.46}$$

where q is the momentum transfer

$$q = 2p\sin\frac{\theta}{2} \,. \tag{9.47}$$

2. Using Eq. (9.46), compute the scattering amplitude and the differential cross section of the particle in the repulsive potential

$$V(r) = V_0 e^{-r^2/a^2} \,. \tag{9.48}$$

▪

▪ **Exercise 9.4 — Scattering in a square-well potential.** A nonrelativistic particle of mass m and momentum p is scattered by the following potential,

$$V(r) = \begin{cases} -V_0 \,, & r < R \,, \\ 0 \,, & r > R \,. \end{cases} \tag{9.49}$$

1. In the first Born approximation, find the differential cross section of the scattering in the potential (9.49). Plot it schematically, indicating angular units.
2. How to extract the value of R from the measured angular distribution of the scattered particles?
3. Assuming the scattered particles to be protons and $R = 5 \cdot 10^{-13}$ *cm*, roughly how high must the energy of the particles be in order for the scattering to be sensitive to R?
4. Compute the total cross section σ of the scattering in the potential (9.49).
   Hint: Rewrite the solid angle element $d\Omega$ through dq with q the momentum transfer.
5. Find σ in the limit of slow scattering, i.e., when the wave length of the particles is much larger than the size of the potential. Explain the observed dependence of σ on the initial momentum p in this limit.
6. Find σ in the opposite limit of fast scattering. What is the dependence on p in this case?

▪

▪ **Exercise* 9.5 — The nucleus form factor.** The study of the scattering of high-energy electrons from nuclei has yielded much interesting information about the charge distributions in nuclei and nucleons. In this exercise we neglect the electron spin and assume that the nucleus remains fixed in space. Let $\rho(\mathbf{x})$ denote the charge density in the nucleus.
Let $f_0(\mathbf{p} \to \mathbf{p}')$ be the scattering amplitude in the first Born approximation for the scattering of an electron from a point nucleus of charge Ze. Let $f(\mathbf{p} \to \mathbf{p}')$ be the scattering amplitude, also in the first Born approximation, for the scattering of an electron from a real nucleus of the same charge. The quantity $F = F(\mathbf{q}^2)$ defined as

$$f(\mathbf{p} \to \mathbf{p}') = F(\mathbf{q}^2) f_0(\mathbf{p} \to \mathbf{p}') \tag{9.50}$$

is called the form factor (it is easily seen that F in fact depends on $\mathbf{p}$ and $\mathbf{p}'$ only through the momentum transfer).

1. Relate the form factor $F(\mathbf{q}^2)$ to the Fourier transform of the charge density $\rho(\mathbf{x})$.
   Indication: Consider the case of spherically symmetric distribution of charge in the nucleus.
2. Figure 9.2 shows some experimental results pertaining to the form factor of the proton. Based on these data, compute the mean-square radius of the proton.
   Hint: Find and use the relation between the mean-square radius and derivative of $F(\mathbf{q}^2)$ with respect to $\mathbf{q}^2$ at $\mathbf{q}^2 = 0$.

▪

▪ **Exercise 9.6 — Applicability condition of the first Born approximation.** On physical grounds, one can expect the accuracy of the Born approximation to increase when the energy of the scattered particles becomes higher or when the interaction term in the Hamiltonian $H = H_0 + V$ becomes weaker. To make this reasoning quantitative, we say that the (first) Born approximation works well if the difference between the asymptotic wave function $\Psi_{in}(\mathbf{x}) = \langle \mathbf{x} | \Psi_{in} \rangle$ and the wave function $\Psi_0(\mathbf{x}) = \langle \mathbf{x} | \Psi_0 \rangle = \langle \mathbf{x} | \Omega_+ | \Psi_{in} \rangle$ is small, in particular

$$|\Psi_{in}(\mathbf{0}) - \Psi_0(\mathbf{0})| \ll |\Psi_{in}(\mathbf{0})| \,. \tag{9.51}$$

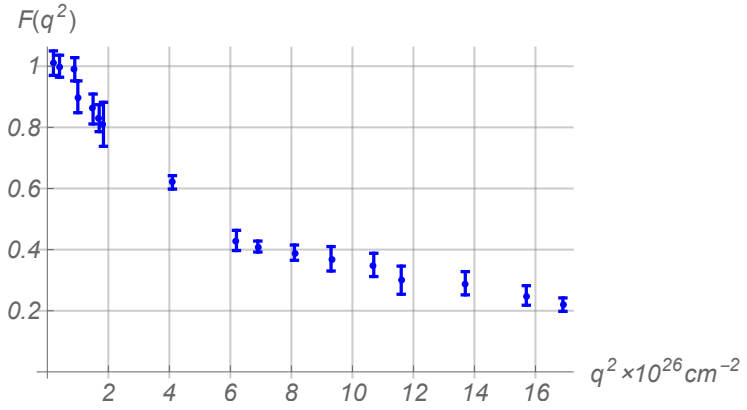


Figure 9.2: The measured form factor as a function of the momentum transfer.

1. Show that for a spherically symmetric potential $V(r)$ the condition (9.51) implies

$$\frac{m}{p}\left|\int_0^\infty dr\, V(r)(1-e^{2ipr})\right| \ll 1\,, \tag{9.52}$$

   where p is the momentum of the particle and m is its mass.
2. As a model example, consider the square well potential,

$$V(r) = \begin{cases} -V_0\,, & r < R\,, \\ 0\,, & r > R\,. \end{cases} \tag{9.53}$$

   Substitute this potential into Eq. (9.52) to obtain an algebraic inequality the quantities m, V_0 and R must satisfy in the limit of slow scattering $pR \ll 1$.
3. Show that this inequality can be rewritten as

$$\sigma \ll 4\pi R^2\,. \tag{9.54}$$

4. Work out the applicability condition for the potential (9.53) in the regime of fast scattering, $pR \gg 1$. Is it stronger or weaker than in the slow scattering limit?
5. Use Eq. (9.52) to derive the applicability conditions for the Yukawa potential,

$$V(r) = \frac{\alpha}{r}e^{-\mu r}\,, \tag{9.55}$$

   in the cases of slow ($p \ll \mu$) and fast ($p \gg \mu$) particles.

▪

▪ **Exercise 9.7 — Towards the inverse scattering problem.** Elastic scattering from some central potential $V(r)$ can be adequately calculated using the first Born approximation. Experimental results give the following qualitative behaviour of the scattering amplitude as a function of the momentum transfer q (see figure 9.3),

i For $q \lesssim q_0$, $|f(q)| \approx f_0$, $\dfrac{|f'(q)|}{q} \approx C$;

ii For $q \gtrsim q_0$, $|f(q)| \sim q^{-N/2}$, $N > 3$.

1. What is the approximate size of the interaction region of the potential $V(r)$?
   Hint: Expand the expression for the scattering amplitude at small q by the powers of qr.

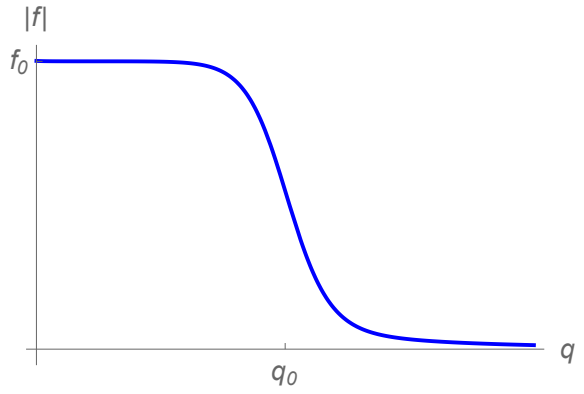


Figure 9.3: Measured behaviour of the scattering amplitude.

2. What is the behaviour of the potential at very small distances?

▪

▪ **Exercise 9.8 — Truncation of the Coulomb potential.** The scattering theory studied in this course is not directly applicable to many important physical situations. In particular, it is not applicable to the Coulomb scattering for which

$$V(r) = \frac{\alpha}{r} \,. \tag{9.56}$$

It is easy to see that a straightforward attempt to compute the Born amplitude with the potential (9.56) results in a divergence. A possible way to produce meaningful results within the conventional scattering theory is to *truncate* the expression (9.56), i.e., to change its behaviour at large distances so that the scattering amplitude becomes well-defined. The answer obtained in this way makes sense as long as any measurement of physical observables with finite accuracy does not depend on a parameter of truncation and on a specific truncation procedure. If this is the case, the result is expected to be consistent with the one computed rigorously.
In this exercise, we consider two ways to improve the asymptotics of the Coulomb potential (9.56) at infinity: the exponential shielding

$$V_\rho(r) = \frac{\alpha}{r} e^{-r/\rho} \,, \tag{9.57}$$

and a sharp cutoff

$$V_\rho(r) = \begin{cases} \dfrac{\alpha}{r} \,, & r \leqslant \rho \,, \\ 0 \,, & r > \rho \,. \end{cases} \tag{9.58}$$

Here ρ is the truncation parameter which is assumed to be finite but arbitrarily large.

1. In the first Born approximation, compute the scattering amplitude $f_1(\mathbf{p} \to \mathbf{p}')$ for the potential (9.57). For which scattering angles does it have a well-defined limit at $\rho \to \infty$?
2. Compute, also in the first Born approximation, the amplitude $f_2(\mathbf{p} \to \mathbf{p}')$ for the potential (9.58). Does it have a limit at $\rho \to \infty$?
3. Show that by taking ρ sufficiently large, the ratio of the two answers $|f_1/f_2|$ can be made arbitrarily close to 1 in any experiment measuring the scattering angle θ with the finite accuracy $\Delta\theta$. In other words, prove that

$$\frac{1}{\Delta\theta} \int_\theta^{\theta+\Delta\theta} d\theta' \left| \frac{f_1(\theta')}{f_2(\theta')} \right| = 1 \,, \quad \theta \neq 0 \,, \quad \rho \gg \rho_0 \,. \tag{9.59}$$

Find ρ_0 as a function of the initial momentum of the particle, the measured scattering angle θ and the systematic error $\Delta\theta$.

4. As another way to convince oneself of the legitimacy of the truncation procedure, consider the out wave packet produced by the potential (9.57) or (9.58),

$$\Psi_{out}(\mathbf{p}) = \Psi_{in}(\mathbf{p}) + \frac{i}{2\pi m}\int d^3\mathbf{p}'\ \delta(E_p - E_{p'}) f_{1,2}(\mathbf{p}\to\mathbf{p}')\Psi_{in}(\mathbf{p}')\ . \tag{9.60}$$

Show that in the limit $q\rho \gg 1$ the difference between f_1 and f_2 makes no contribution to $\Psi_{out}(\mathbf{p})$.

▪

▪ **Exercise* 9.9 — Yukawa potential beyond the first Born approximation.** Consider the Yuakawa potential

$$V(r) = \frac{\alpha}{r}e^{-\mu r}\ . \tag{9.61}$$

1. Calculate the second order in α term of the scattering amplitude for the potential (9.61). *Hint:* To compute the angular part of the amplitude, use Feynman's trick:

$$\frac{1}{ab} = \frac{1}{2}\int_{-1}^{1} dz \left(a\frac{1+z}{2} + b\frac{1-z}{2}\right)^{-2}\ . \tag{9.62}$$

2. Find the differential cross section $d\sigma/d\Omega$ to the third order in α.
3. What is the width of the forward diffraction peak, that is, of the region in which the differential cross section shows no dependence on the scattering angle? Write $d\sigma/d\Omega$ in this region.
4. To test the applicability of the *first* Born approximation, find the ratio of the α^3- to the α^2-contributions to $d\sigma/d\Omega$ and require it to be small. Find what conditions this requirement imposes on the parameters of the potential and particle's momentum p
   - in the slow scattering regime, $p \ll \mu$,
   - in the fast scattering regime, $p \gg \mu$.

   Compare with the results of p. 5 Exercise 9.6.

▪

Lecture 10

> Stationary scattering states; S-matrix as T-product.

10.1 Scattering amplitude via stationary scattering states

In this section, we discuss another method of finding the scattering amplitude. It utilizes eigenstates of the full Hamiltonian H. Denote

$$|\mathbf{p}_\pm\rangle = \Omega_\pm |\mathbf{p}\rangle \,, \tag{10.1}$$

where $|\mathbf{p}\rangle$ are momentum eigenstates of the free Hamiltonian. In lecture 8 it was shown that $|\mathbf{p}_\pm\rangle$ are eigenstates of H with the eigenvalues $E_p = p^2/2m$. Here we will show that the wave function $\langle \mathbf{x}|\mathbf{p}_+\rangle$ has the following asymptotics at $r \to \infty$:

$$\langle \mathbf{x}|\mathbf{p}_+\rangle = \frac{1}{(2\pi)^{3/2}} \left[e^{i\mathbf{p}\cdot\mathbf{x}} + f\left(p\frac{\mathbf{x}}{r} \leftarrow \mathbf{p}\right) \frac{e^{ipr}}{r} \right] , \tag{10.2}$$

where $p = |\mathbf{p}|$, $r = |\mathbf{x}|$, and f is the scattering amplitude. Eq. (10.2) suggests the following algorithm of determining f:

- write the time-independent Schroedinger equation;
- find its general solution;
- select particular solutions obeying the asymptotics (10.2);
- read off the scattering amplitude.

This algorithm is analogous to the investigation of scattering in one-dimensional quantum mechanics. Indeed, when one deals with the potential scattering in one dimension, one looks for the solutions ψ of the stationary Schroedinger equation with the asymptotic behaviour (let the incident wave approach the potential from the left)

$$\begin{aligned} &\psi \to e^{ipx} + R\, e^{-ipx} \,, \quad x \to -\infty \,, \\ &\psi \to D\, e^{ipx} \,, \quad x \to +\infty \,. \end{aligned} \tag{10.3}$$

Here R is the reflection coefficient, and D is the transmission coefficient which can be identified with the matrix element of the one-dimensional S-matrix (see Exercise 7.4). Similarly to the first of Eqs. (10.3), the first term in the r.h.s. of Eq. (10.2) represents the incident plane wave, and the second — the spherical wave spreading out from the scattering center.

It is important to note that neither the plane waves $|\mathbf{p}\rangle$ nor the stationary states $|\mathbf{p}_\pm$ can represent actual scattering states realized in experiment. Their role is to provide a convenient basis in the

Hilbert space $\mathscr{H}$, with respect to which one can expand the in and out-asymptotic states, and the states at the moment of interaction, respectively. For example, let the in-state $|\phi\rangle$ admit the following decomposition into the plane waves:

$$|\phi\rangle = \int d^3\mathbf{p}\,\phi(\mathbf{p})|\mathbf{p}\rangle\ . \tag{10.4}$$

Then, the actual state at the moment of interaction, $t=0$, is

$$\Omega_+|\phi\rangle = \int d^3\mathbf{p}\,\phi(\mathbf{p})\Omega_+|\mathbf{p}\rangle = \int d^3\mathbf{p}\,\phi(\mathbf{p})|\mathbf{p}_+\rangle\ . \tag{10.5}$$

In other words, the actual state $\Omega_+|\phi\rangle$ has the same expansion in terms of $|\mathbf{p}_+\rangle$ as does its in-asymptote $|\phi\rangle$ in terms of $|\mathbf{p}\rangle$. The similar statement holds for the out asymptote.

Recall that Ω_+ maps $\mathscr{H}$ onto the subspace $\mathscr{R}$ of scattering states. According to Eq. (10.5), any scattering state can be expanded in terms of $|\mathbf{p}_+\rangle$. Furthermore, we have

$$\begin{aligned}\langle\mathbf{p}'_+|\mathbf{p}_+\rangle &= \langle\mathbf{p}'|\Omega_+^\dagger\Omega_+|\mathbf{p}\rangle = \langle\mathbf{p}'|\mathbf{p}\rangle \\ &= \delta^{(3)}(\mathbf{p}'-\mathbf{p})\ .\end{aligned} \tag{10.6}$$

This shows that $|\mathbf{p}_+\rangle$ form an orthonormal basis in $\mathscr{R}$. Since $\mathscr{H}=\mathscr{R}\oplus\mathscr{B}$, where $\mathscr{B}$ is spanned by the bound states (say, $|n\rangle$), we conclude that $|\mathbf{p}_+\rangle$ together with the bound states form an orthonormal basis in $\mathscr{H}$. Of course, the same holds for $|\mathbf{p}_-\rangle$. To summarize,

$$\begin{aligned}1 &= \int d^3\mathbf{p}\,|\mathbf{p}\rangle\langle\mathbf{p}| \\ &= \int d^3\mathbf{p}\,|\mathbf{p}_+\rangle\langle\mathbf{p}_+| + \sum_n |n\rangle\langle n| \\ &= \int d^3\mathbf{p}\,|\mathbf{p}_-\rangle\langle\mathbf{p}_-| + \sum_n |n\rangle\langle n|\ .\end{aligned} \tag{10.7}$$

Let us now prove Eq. (10.2). By using Eq. (8.27), we can write the vector $|\mathbf{p}_+\rangle$ in the form

$$|\mathbf{p}_+\rangle = |\mathbf{p}\rangle + G(E_p+i\varepsilon)V\,|\mathbf{p}\rangle\ . \tag{10.8}$$

Next, using Eq. (9.9) we have, in the x-representation,

$$\begin{aligned}\langle\mathbf{x}|\mathbf{p}_+\rangle &= \langle\mathbf{x}|\mathbf{p}\rangle + \langle\mathbf{x}|G_0(E_p+i\varepsilon)T(E_p+i\varepsilon)|\mathbf{p}\rangle \\ &= \langle\mathbf{x}|\mathbf{p}\rangle + \int d^3\mathbf{x}'d^3\mathbf{p}'\,\langle\mathbf{x}|G_0(E_p+i\varepsilon)|\mathbf{x}'\rangle\,\langle\mathbf{x}'|\mathbf{p}'\rangle\,\langle\mathbf{p}'|T(E_p+i\varepsilon)|\mathbf{p}\rangle \\ &= \langle\mathbf{x}|\mathbf{p}\rangle + \int d^3\mathbf{x}'d^3\mathbf{p}'\langle\mathbf{x}'|\mathbf{p}'\rangle\langle x|G_0(E_p+i\varepsilon)|\mathbf{x}'\rangle\left[-\frac{f(\mathbf{p}'\leftarrow\mathbf{p})}{(2\pi)^2 m}\right] \\ &= \frac{1}{(2\pi)^{3/2}}\left[e^{i\mathbf{p}\cdot\mathbf{x}} - \frac{1}{(2\pi)^2 m}\int d^3\mathbf{x}'d^3\mathbf{p}'e^{i\mathbf{p}'\cdot\mathbf{x}'}f(\mathbf{p}'\leftarrow\mathbf{p})\langle x|G_0(E_p+i\varepsilon)|\mathbf{x}'\rangle\right]\ .\end{aligned} \tag{10.9}$$

To proceed further, we use the explicit form of free particle Green's function (see Exercise 8.2),

$$\langle\mathbf{x}|G_0(E+i\varepsilon)|\mathbf{x}'\rangle = -\frac{m}{2\pi|\mathbf{x}-\mathbf{x}'|}e^{ip|\mathbf{x}-\mathbf{x}'|-\varepsilon|\mathbf{x}-\mathbf{x}'|}\ . \tag{10.10}$$

At large $|\mathbf{x}|$, one can expand

$$\begin{aligned}|\mathbf{x}-\mathbf{x}'| &= \left|r^2+r'^2-2\mathbf{x}\cdot\mathbf{x}'\right|^{1/2} \\ &= r\left[1-\frac{\mathbf{x}\cdot\mathbf{x}'}{r^2}+O\left(\frac{1}{r^2}\right)\right] \\ &\approx r-\frac{\mathbf{x}}{r}\cdot\mathbf{x}'\ .\end{aligned} \tag{10.11}$$

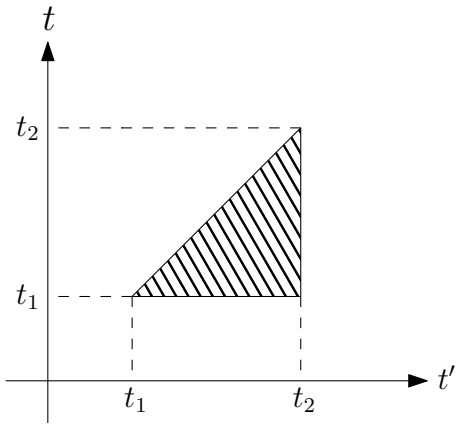


Figure 10.1: The area of integration in the 2nd term of the expansion (10.18).

Using Eqs. (10.10), (10.11) and integrating over $\mathbf{x}'$ yields

$$\begin{aligned}\langle \mathbf{x}|\mathbf{p}_+\rangle &= \frac{1}{(2\pi)^{3/2}}\left[e^{i\mathbf{p}\cdot\mathbf{x}} + \frac{1}{(2\pi)^3}\int d^3\mathbf{x}' d^3\mathbf{p}' f(\mathbf{p}'\leftarrow\mathbf{p}) e^{i\mathbf{p}'\cdot\mathbf{x}'}\frac{1}{r}e^{ipr+ip\mathbf{x}\cdot\mathbf{x}'/r}\right] \\ &= \frac{1}{(2\pi)^{3/2}}\left[e^{i\mathbf{p}\cdot\mathbf{x}} + \int d^3\mathbf{p}'\delta^{(3)}\left(\mathbf{p}' - p\frac{\mathbf{x}}{r}\right) f(\mathbf{p}'\leftarrow\mathbf{p})\frac{1}{r}e^{ipr}\right] \\ &= \frac{1}{(2\pi)^{3/2}}\left[e^{i\mathbf{p}\cdot\mathbf{x}} + f\left(p\frac{\mathbf{x}}{r}\leftarrow\mathbf{p}\right)\frac{1}{r}e^{ipr}\right],\end{aligned} \tag{10.12}$$

which completes the derivation of Eq. (10.2).

10.2 S-matrix as T-product

The discussion of scattering theory would be incomplete without yet another representation of the S-matrix that is particularly useful in quantum field theory:

$$S = T\exp\left(-i\int_{-\infty}^{\infty} dt V(t)\right). \tag{10.13}$$

Here T is the so-called time-ordering operator, or T-product, whose effect is reordering operators on its right chronologically, e.g.,

$$TV(t_1)V(t_2) = \theta(t_1-t_2)V(t_1)V(t_2) + \theta(t_2-t_1)V(t_2)V(t_1). \tag{10.14}$$

To prove Eq. (10.13), we take the definition (7.15) of S-matrix and differentiate it with respect to t_1:

$$\begin{aligned}\frac{\partial}{\partial t_1}S(t_1,t_2) &= -iU_0^\dagger(t_1)(H-H_0)U_0(t_1)S(t_1,t_2) \\ &= -iV(t_1)S(t_1,t_2),\end{aligned}$$

where $V(t)$ is the interaction Hamiltonian in the interaction picture. Since $S(t_2,t_2)=1$, integrating back with respect to t_1 gives

$$S(t_1,t_2) = 1 - i\int_{t_2}^{t_1} dt V(t)S(t,t_2). \tag{10.15}$$

This equation can be solved by iterations. One can take $S = 1$ initially, which amounts to neglecting the interaction. Substituting to the r.h.s. of Eq. (10.15) gives the first iteration,

$$S = 1 - i\int_{t_2}^{t_1} dtV(t)\ . \tag{10.16}$$

Repeating the substitution produces the second iteration,

$$S = 1 - i\int_{t_2}^{t_1} dtV(t) + (-i)^2\int_{t_2}^{t_1} dtV(t)\int_{t_2}^{t} dt'V(t')\ , \tag{10.17}$$

and so on. Note that in the second term in the r.h.s. of Eq. (10.17) the integration is over the triangular area in the plane spanned by t_1 and t_2, see figure 10.1. Such area is often referred to as (2-dimensional) "simplex". We can, therefore, write

$$S = \sum_{n=0}^{\infty} S_n\ , \tag{10.18}$$

where

$$S_n = (-i)^n\int_{t_2}^{t_1} dtV(t)\int_{t_2}^{t} dt'V(t')\int_{t_2}^{t'} dt''V(t'')\ldots \tag{10.19}$$

For potential scattering, the expansion (10.18) is equivalent to the Born series, but, unlike the latter, it admits a more straightforward generalization to other theories and, in particular, to quantum field theory. The integration in Eq. (10.19) is performed over the n-dimensional simplex, $t_1 > t > t' > ... > t_2$. These limits of integration are reproduced automatically if one introduces the T-product:

$$S_n = (-1)^n\frac{1}{n!}\int_{t_1}^{t_2} dt\int_{t_1}^{t_2} dt'\int_{t_1}^{t_2} dt''\ldots(TV(t)V(t')V(t'')\ldots)\ . \tag{10.20}$$

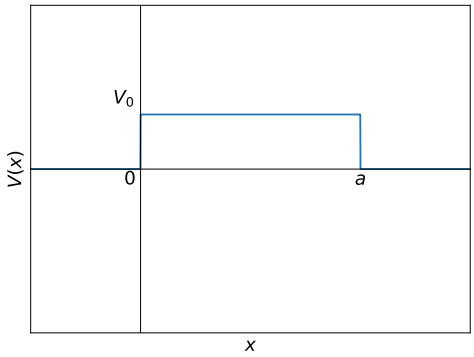
In the last expression, the integration is performed over the n-dimensional cube. The series in the expansion of S can now be easily summed up to yield Eq. (10.13).

Lecture 11

> Scattering phase shift; free spherical waves; partial waves in the first Born approximation.

11.1 Scattering phase shift and central potential

Consider a square potential in 1D



and an incoming (from the left side) plane wave with energy $E > V_0$. The outgoing wave, on the right side, is also a plane wave, albeit with a phase shift δ, whose actual value depends on the details of the potential (here, a and V_0) (see Figure **??**).

The phase difference is of little importance for the problem of 1D barrier tunneling because it is not measurable: the incoming and outgoing waves propagate in different regions (on the left and right sides of the potential barrier, respectively), and as such do not form an interference pattern that could be detected in experiments.

Let us now consider the 3D case. From the previous lectures, the scattering states in the asymptotic limit can be written as:

$$\langle \mathbf{r}|\mathbf{p}_{\pm}\rangle \underset{r\to\infty}{\to} \frac{1}{(2\pi)^{3/2}} \left(\underbrace{e^{i\mathbf{p}\cdot\mathbf{r}}}_{\text{in-state}} + \underbrace{f(p\frac{\mathbf{r}}{r} \leftarrow \mathbf{p})\frac{e^{ipr}}{r}}_{\text{scattered wave}} \right). \tag{11.1}$$

Contrary to the one dimensional case, the in-state and scattered wave now interfere, thus the phase shift becomes important.

A large class of scattering potentials are central (i.e. spherically symmetric). To study these, consider a plane wave propagating along the z axis. The wave function can be written as:

$$\psi \sim e^{ip_z z} + \frac{f(\theta)}{r} e^{ipr}. \tag{11.2}$$

In the case of central potentials, stationary states have well defined angular momentum: indeed, the Hamiltonian commutes with $\hat{L}_z$ and $\hat{L}^2$ (cf. Quantum Physics I/II courses). Recall that in spherical coordinates:

$$\begin{cases} \hat{L}_z = -i\hbar \frac{\partial}{\partial \varphi} \\ \hat{L}^2 = -\hbar^2 \left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial}{\partial \phi^2} \right) \end{cases} \tag{11.3}$$

These two operators commuting with the Hamiltonian induce two new quantum numbers, l and m. In particular, the common basis of eigenvectors of $\hat{H}$, $\hat{L}^2$ and $\hat{L}_z$ are partial waves $\varphi_{klm}(\mathbf{r})$, with eigenvalues $\frac{\hbar^2 k^2}{2m}$, $l(l+1)\hbar^2$ and $m\hbar$ respectively. Furthermore, the partial waves can be factorized into the radial and angular parts

$$\varphi_{klm}(\mathbf{r}) = R_{kl}(r) Y_l^m(\theta, \varphi), \tag{11.4}$$

with Y_l^m being the spherical harmonic functions.

At $r \to \infty$, partial waves converge to common eigenfunctions of $\hat{H}_0$, $\hat{L}^2$ and $\hat{L}_z$. The wavefunctions φ^0_{klm} are spherical harmonics, but the radial part is a result of interference of incoming and outgoing waves with a certain phase difference.

11.2 Free spherical waves

Consider the special case of a free particle. We are going to show that the free spherical waves are written as

$$\varphi^0_{klm}(\mathbf{r}) = \sqrt{\frac{2k}{\pi}} j_l(kr) Y_l^m(\theta, \varphi) \tag{11.5}$$

where $j_l(\rho)$ are the spherical Bessel functions, defined as

$$j_l(\rho) = (-1)^l \rho^l \left(\frac{1}{\rho} \frac{\mathrm{d}}{\mathrm{d}\rho} \right)^l \frac{\sin\rho}{\rho}. \tag{11.6}$$

See the exercises for the properties of these special functions.

Proof

Following the standard approach (see Quantum Physics I/II courses), one can start with the radial equation

$$\left[-\frac{\hbar^2}{2m} \frac{1}{r} \frac{\mathrm{d}^2}{\mathrm{d}r^2} r + \frac{l(l+1)\hbar^2}{2mr^2} \right] R_{kl}(r) = E_{kl} R_{kl}(r). \tag{11.7}$$

Performing the change of variable $R_{kl} = u_{kl}/r$ gives

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} + \frac{2mE_{kl}}{\hbar^2} \right] u_{kl}(r) = 0, \tag{11.8}$$

with the boundary condition $u_{kl}(0) = 0$. Recall that $E_{kl} = \frac{\hbar^2 k^2}{2m}$. In the large r limit, the second term $l(l+1)/r^2$ vanishes, leading to:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2\right] u_{kl}(r) \underset{r\to\infty}{\approx} 0 \tag{11.9}$$

The solution is a linear combination of e^{ikr} and e^{-ikr}, with the boundary condition $u_{kl}(0) = 0$ making it unique.

For example, the $l = 0$ case can be easily solved:

$$u_{k0}(r) = a_k \sin(kr), \tag{11.10}$$

with $a_k = \sqrt{\frac{2}{\pi}}$. Since $Y_0^0 = \frac{1}{\sqrt{4\pi}}$:

$$\varphi^0_{k00}(r) = \sqrt{\frac{2k^2}{\pi}} \frac{1}{\sqrt{4\pi}} \frac{\sin(kr)}{kr}. \tag{11.11}$$

The solution of the radial equation for $l > 0$ can be obtained by recurrence

$$\hat{P}_+ \varphi^0_{kll}(r) \propto \varphi^0_{k(l+1)(l+1)}(r) \tag{11.12}$$

with $\hat{P}_+ = \hat{P}_x + i\hat{P}_y$, and similarly

$$\hat{L}_\pm \varphi^0_{klm}(r) \propto \varphi^0_{kl(m\pm1)}(r). \tag{11.13}$$

For the full derivation, see Complement $\mathrm{A_{VIII}}$ of Cohen-Tannoudji's *Quantum Physics*.

We thus have

$$\varphi^0_{kll}(r) \propto \hat{P}_+ \varphi^0_{k00}(r) \propto \hat{P}_+ \frac{\sin(kr)}{kr}. \tag{11.14}$$

Now, we would like to obtain an explicit expression for u_{kll}. We can write the ladder operator $\hat{P}_+$ in the x-representation, pointing out that it is applied to a function depending purely on r:

$$\hat{P}_+ f(\vec{r}) = -i\hbar \left(\frac{\partial f}{\partial x} + i\frac{\partial f}{\partial x}\right) = -i\hbar \left(\frac{x}{r} + i\frac{y}{r}\right) \frac{\mathrm{d}}{\mathrm{d}r} f(r) = -i\hbar \sin\theta e^{i\varphi} \frac{\mathrm{d}}{\mathrm{d}r} f(r). \tag{11.15}$$

Thus, we obtain:

$$\varphi^0_{k11}(\vec{r}) \propto \underbrace{\sin\theta e^{i\varphi}}_{Y_1^1(\theta,\varphi)} \left(\frac{\cos kr}{kr} - \frac{kr}{(kr)^2}\right). \tag{11.16}$$

Similarly, we can apply $\hat{L}_-$ to obtain $\varphi^0_{k10}(\vec{r})$ and $\varphi^0_{k1-1}(\vec{r})$.

To compute explicitly φ^0_{kll} for higher l, see first that $[\hat{P}_+, \hat{X} + i\hat{Y}] = 0$. Thus

$$\varphi^0_{k22}(\vec{r}) \propto \hat{P}_+^2 \frac{\sin kr}{kr} = \hat{P}_+ \frac{x+iy}{r} \frac{\mathrm{d}}{\mathrm{d}r} \frac{\sin kr}{kr} = (x+iy)\hat{P}_+ \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\frac{\sin kr}{kr} \tag{11.17}$$

$$= (x+iy)^2 \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left[\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\frac{\sin kr}{kr}\right] = (x+iy)^2 \left(\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right)^2 \frac{\sin kr}{kr}. \tag{11.18}$$

It is easy to infer the general case from here:

$$\varphi^0_{kll}(\vec{r}) \propto (x+iy)^l \left(\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right)^l \frac{\sin kr}{kr}. \tag{11.19}$$

The first factor can be understood as the angular part

$$(x+iy)^l = r^l(\sin\theta)^l e^{il\varphi} \propto Y_l^l(\theta,\varphi). \tag{11.20}$$

The radial part can be written with the spherical Bessel function of order l

$$j_l(\rho) := (-1)^l \rho^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{\sin\rho}{\rho}, \tag{11.21}$$

which leads to the actual expression for $\varphi^0_{klm}(\vec{r})$

$$\varphi^0_{klm}(\vec{r}) = R_{kl}(r)Y_m^l(\theta,\varphi) = \sqrt{\frac{2k^2}{\pi}}\, j_l(kr)Y_m^l(\theta,\varphi). \tag{11.22}$$

The prefactor is responsible for normalization.

Remark

The free spherical waves form an orthonormal basis set

$$\langle\varphi^0_{klm}|\varphi^0_{k'l'm'}\rangle = \delta(k-k')\delta_{ll'}\delta_{mm'} \tag{11.23}$$

$$\int_0^\infty \mathrm{d}k \sum_{l=0}^{\infty}\sum_{m=-l}^{l} |\varphi^0_{klm}\rangle\langle\varphi^0_{klm}| = 1 \tag{11.24}$$

Asymptotic property for $\rho \to 0$

First, we would like to compute the probability density for a free spherical wave (equation 11.22). Consider an infinitesimal solid angle $(\mathrm{d}\theta,\mathrm{d}\varphi)$ centered around (θ_0,φ_0). The probability of finding the particle in this solid angle, for a radius comprised between r and $r+\mathrm{d}r$ is

$$\frac{2(kr)^2}{\pi}|j_l(kr)|^2|Y_m^l(kr)|^2\sin\theta_0\ \mathrm{d}r\mathrm{d}\theta\mathrm{d}\varphi. \tag{11.25}$$

This implies that in the limit of small radius $\rho = kr$ (see exercises), the spherical Bessel functions can be written as

$$j_l(\rho) \underset{\rho\to 0}{\to} \frac{\rho^l}{(2l+1)!!}. \tag{11.26}$$

It means that the probability density behaves like r^{2l+2} as $r \to 0$. One would expect that for larger and larger l, the probability density remains small in a ever increasing neighborhood of $r = 0$. Quantitatively, the position of the first peak of the probability density scales with l as $\rho_0 \sim \sqrt{l(l+1)}$ (see figure 11.1). This implies that the free spherical wave $|\varphi^0_{klm}\rangle$ is unaffected by what happens within a radius $r_0(k) = \frac{1}{k}\sqrt{l(l+1)}$.

Asymptotic property for $\rho \to \infty$

Again, see the exercise for the actual derivation

$$j_l(\rho) \underset{\rho\to\infty}{\sim} \frac{1}{\rho}\sin(\rho - l\frac{\pi}{2}). \tag{11.27}$$

Consequently,

$$\varphi^0_{klm}(\mathbf{r}) \underset{r\to\infty}{\sim} -\sqrt{\frac{2k^2}{\pi}}Y_l^m(\theta,\varphi)\frac{e^{-ikr}e^{il\frac{\pi}{2}} - e^{ikr}e^{-il\frac{\pi}{2}}}{2ikr}, \tag{11.28}$$

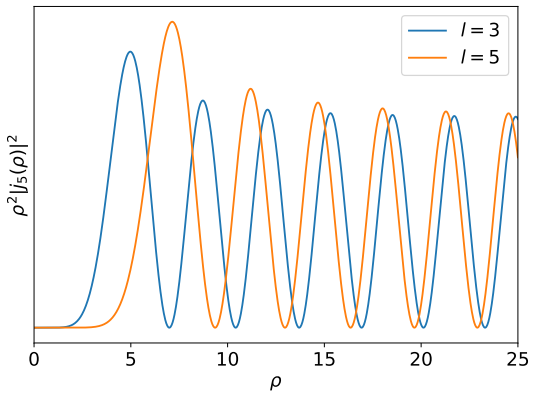


Figure 11.1: Radial probability for free spherical waves with $l = 3$ and $l = 5$.

which can be interpreted as the superposition of an incoming and outgoing wave, respectively, of the form $\frac{e^{\pm ikr}}{r}$ with a phase difference $l\pi$.

We can now express plane waves in terms of free spherical waves ($\vec{p} = \vec{k} = |0,0,k\rangle$)

$$\langle \vec{r}|\vec{k}\rangle = \left(\frac{1}{2\pi}\right)^{3/2} e^{ikz} \tag{11.29}$$

$|0,0,k\rangle$ represents a state of well-defined energy and momentum ($E = \frac{\hbar^2 k^2}{2m}$; $\vec{p}$ directed along Oz with modulus $\hbar k$). Now

$$e^{ikz} = e^{ikr\cos\theta} \tag{11.30}$$

is independent of φ; since L_z corresponds to $\frac{\hbar}{i}\frac{\partial}{\partial\varphi}$ in the x-representation, the ket $|\vec{k}\rangle$ is also an eigenvector of L_z with the eigenvalue zero:

$$L_z|\vec{k}\rangle = 0. \tag{11.31}$$

Here, we can write $|\vec{k}\rangle$ as:

$$|\vec{k}\rangle = \int_0^\infty dk' \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} |\varphi^{(0)}_{k'lm}\rangle\langle\varphi^{(0)}_{k'lm}|\vec{k}\rangle. \tag{11.32}$$

Since $|0,0,k\rangle$ and $|\varphi^{(0)}_{klm}\rangle$ are two eigenstates of H_0, these states are orthogonal if the corresponding eigenvalues are different; their scalar product is therefore proportional to $\delta(k'-k)$. Similarly, these states are both eigenstates of L_z and their scalar product is proportional to δ_{m0}. Eq.11.32 therefore takes the form

$$|\vec{k}\rangle = \sum_{l=0}^{\infty} c_{kl}|\varphi^{(0)}_{k,l,0}\rangle. \tag{11.33}$$

The coefficients c_{kl} can be calculated explicitly. Thus, we obtain:

$$\begin{aligned} e^{ikz} &= \sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)}\, j_l(kr)\, Y_l^0(\theta) \\ &= \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta) \end{aligned} \tag{11.34}$$

A state of well-defined linear momentum is therefore formed by the superposition of states corresponding to all possible angular momenta.

The spherical harmonic $Y_l^0(\theta)$ is proportional to the Legendre polynomial $P_l(\cos\theta)$:

$$Y_l^0(\theta) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta). \tag{11.35}$$

Hence, expansion Eq(11.34) is often written in the form:

$$e^{ikz} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta). \tag{11.36}$$

11.3 Partial waves in the potential $V(r)$

We are now going to study the eigenfunctions common to H (the total Hamiltonian), L^2 and L_z; that is, the partial waves $\varphi_{klm}(r)$.

Let us now introduce our potential $V(r)$. For any central potential $V(r)$, the partial waves $\varphi_{klm}(r)$ are of the form

$$\varphi_{klm}(r) = R_{kl}(r) Y_l^m(\theta,\varphi) = \frac{1}{r} u_{kl}(r) Y_l^m(\theta,\varphi), \tag{11.37}$$

where $u_{kl}(r)$ is the solution of the radial equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r) \right] u_{kl}(r) = \frac{\hbar^2 k^2}{2\mu} u_{kl}(r) \tag{11.38}$$

satisfying the boundary condition at the origin

$$u_{k,l}(0) = 0. \tag{11.39}$$

We can view this as an effective 1D problem, where a particle of mass m in effective potential:

$$V_{\text{eff}}(r) = \begin{cases} V(r) + \frac{l(l+1)\hbar^2}{2\mu r^2}, & \text{for } r > 0 \\ \infty. & \text{for } r < 0 \end{cases} \tag{11.40}$$

For large r, Eq(11.38) reduces to

$$\left[\frac{d^2}{dr^2} + k^2 \right] u_{kl}(r) \underset{r\to\infty}{\sim} 0 \tag{11.41}$$

with the general solution

$$u_{kl}(r) \underset{r\to\infty}{\sim} A e^{ikr} + B e^{-ikr}. \tag{11.42}$$

Since $u_{kl}(r)$ must satisfy condition Eq(11.39), constants A and B cannot be arbitrary. In the equivalent 1D problem, equation Eq(11.39) is related to the fact that the potential is infinite for negative r, and expression Eq(11.42) represents the superposition of an "incident" plane wave e^{-ikr} coming from the right (along the axis on which the fictitious particle being studied moves) and a "reflected" plane wave e^{ikr} propagating from left to right.

Since there can be no "transmitted" wave ($V_{\text{eff}} = \infty$ at $r < 0$), the "reflected" current must be equal to the "incident" current. Thus, we see that condition Eq(11.39) implies that, in the asymptotic expression Eq(11.42)

$$|A| = |B| \tag{11.43}$$

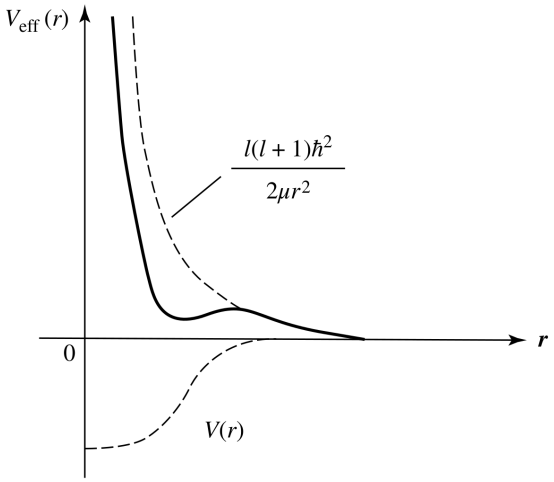


Figure 11.2: The effective potential $V_{\text{eff}}(r)$ is sum of the potential $V(r)$ and the centrifugal term $\frac{l(l+1)\hbar^2}{2mr^2}$.

Hence,

$$u_{kl}(r) \underset{r\to\infty}{\sim} |A| \left[e^{ikr} e^{i\varphi_A} + e^{-ikr} e^{i\varphi_B} \right], \tag{11.44}$$

which can be written in the form

$$u_{kl}(r) \underset{r\to\infty}{\sim} C \sin(kr - \beta_l) \tag{11.45}$$

Since for $V(r) = 0$, $\beta_l = l\pi/2$, we can write

$$u_{k,l}(r) \underset{r\to\infty}{\sim} C \sin\left(kr - l\frac{\pi}{2} + \delta_l \right). \tag{11.46}$$

The quantity δ_l is called the *phase shift* of the partial wave $\varphi_{klm}(r)$; it obviously depends on k, that is, on energy.

Taking Eq(11.37) and Eq(11.46) into account, we can write the expression for the asymptotic behavior of $\varphi_{klm}(r)$ in the form

$$\begin{aligned} \varphi_{klm}(r) &\underset{r\to\infty}{\sim} C \frac{\sin(kr - l\pi/2 + \delta_l)}{r} Y_l^m(\theta,\varphi) \\ &\underset{r\to\infty}{\sim} -CY_l^m(\theta,\varphi) \frac{e^{-ikr} e^{i(l\pi/2-\delta_l)} - e^{ikr} e^{-i(l\pi/2-\delta_l)}}{2ikr} \end{aligned} \tag{11.47}$$

We can see that the partial wave $\varphi_{klm}(r)$, like a free spherical wave, results from the superposition of an incoming wave and an outgoing wave.

In order to develop the comparison between partial waves and free spherical waves in detail, we can modify the incoming wave of Eq(11.47) so as to make it identical to the one in free spherical wave. To do this, we define a new partial wave $\tilde{\varphi}_{klm}(r)$ by multiplying $\varphi_{klm}(r)$ by $e^{i\delta_l}$ (this global phase factor has no physical importance) and by choosing constant C in such a way that

$$\tilde{\varphi}_{klm}(r) \underset{r\to\infty}{\sim} -Y_l^m(\theta,\varphi) \frac{e^{-ikr} e^{il\pi/2} - e^{ikr} e^{-il\pi/2} e^{2i\delta_l}}{2ikr}. \tag{11.48}$$

As this incoming wave approaches the zone of influence of the potential, it is more and more perturbed by this potential. When, after turning back, it is transformed into an outgoing wave, it

has an accumulated a phase shift of $2\delta_l$ relative to the free outgoing wave that would have resulted if the potential $V(r)$ had been identically zero. The factor $e^{2i\delta_l}$ (which varies with l and k) thus summarizes the total effect of the potential on a particle of angular momentum l. This is the physical interpretation differential cross section in terms of the phase shift.

Phase shifts characterize the modifications, caused by the potential, of the asymptotic behavior of stationary states with well-defined angular momentum. Knowing them should therefore allow us to determine the cross section. To demonstrate this, all we must do is express the stationary scattering state $\Psi_k^{(\text{scatt})}(\mathbf{r})$ in terms of partial waves and calculate the scattering amplitude in this way.

Our approach is to find the linear superposition of partial waves with asymptotic behavior

$$\Psi_k^{scatt}(\vec{r}) \underset{r\to\infty}{\sim} e^{ikr} + f_k(\theta)\frac{e^{ikr}}{r} \tag{11.49}$$

Since the stationary scattering state is an eigenstate of the Hamiltonian H, the expansion of $\Psi_k^{(\text{scatt})}(\mathbf{r})$ involves only partial waves having the same energy $\hbar^2k^2/2m$. Note also that, in the case of a central potential $V(r)$, the scattering problem we are studying is symmetrical with respect to rotation around the Oz axis defined by the incident beam. Consequently, the stationary scattering wave function $\Psi_k^{(\text{scatt})}(\vec{r})$ is independent of the azimuthal angle φ, so that its expansion includes only partial waves for which m is zero. Finally, we have an expression of the form

$$\Psi_k^{(\text{scatt})}(\vec{r}) = \sum_{l=0}^{\infty} c_l \tilde{\varphi}_{kl0}(r). \tag{11.50}$$

The problem thus consists of finding the coefficients c_l.

When $V(r)$ is identically zero, the function $\Psi_k^{(\text{scatt})}(\vec{r})$ reduces to the plane wave e^{ikz}, and the partial waves become free spherical waves $\varphi_{klm}^{(0)}(r)$. For non-zero $V(r)$, $\Psi_k^{(\text{scatt})}(\vec{r})$ includes a diverging scattered wave as well as a plane wave. Furthermore, we have seen that $\tilde{\varphi}_{kl0}(r)$ differs from $\varphi_{kl0}^{(0)}(r)$ in its asymptotic behavior only by the presence of the outgoing wave, which has the same radial dependence as the scattered wave. We should therefore expect that the coefficients c_l of the expansion will be the same as those in formula Eq(11.34), that is

$$\Psi_k^{(\text{scatt})}(\vec{r}) = \sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)}\tilde{\varphi}_{kl0}(r). \tag{11.51}$$

Here, the right-hand side is a superposition of eigenstates of H having the same energy $\hbar^2k^2/2m$; consequently, this superposition remains a stationary state. Therefore, all we must do is make sure that the asymptotic behavior of this equation is correct. In order to do this, we can do the following

$$\sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)}\tilde{\varphi}_{kl0}(r) \underset{r\to\infty}{\sim} -\sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)}Y_l^0(\theta) \times \frac{1}{2ikr}\left[e^{-ikr}e^{i\frac{l\pi}{2}} - e^{ikr}e^{-i\frac{l\pi}{2}}e^{2i\delta_l}\right]. \tag{11.52}$$

In order to bring out the asymptotic behavior of Eq(11.34), we use the following property

$$\begin{aligned} e^{2i\delta_l} &= \cos 2\delta_l + i\sin 2\delta_l \\ &= 2\cos^2\delta_l - 1 + 2i\sin\delta_l\cos\delta_l \\ &= -2\sin^2\delta_l + 1 + 2i\sin\delta_l\cos\delta_l \\ &= 1 + 2ie^{i\delta_l}\sin\delta_l \end{aligned} \tag{11.53}$$

and, regrouping the terms that are independent of δ_l, obtain

$$\sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)}\tilde{\varphi}_{kl0}(r) \underset{r\to\infty}{\sim} -\sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)}Y_l^0(\theta) \times \left[\underbrace{\frac{e^{-ikr}e^{i\pi/2} - e^{ikr}e^{-i\pi/2}}{2ikr}}_{\text{phase wave}} - e^{ikr}\frac{1}{k}e^{-i\frac{l\pi}{2}}e^{i\delta_l}\sin\delta_l \right]. \tag{11.54}$$

In the first term of the right-hand side, the asymptotic expansion of the plane wave e^{ikz}, and we obtain finally

$$\sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)}\tilde{\varphi}_{kl0}(r) \underset{r\to\infty}{\sim} e^{ikz} + f_k(\theta)\frac{e^{ikr}}{r} \tag{11.55}$$

with

$$f_k(\theta) = \frac{1}{k}\sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)}e^{i\delta_l}\sin\delta_l\, Y_l^0(\theta). \tag{11.56}$$

We have obtained the desired form and have found at the same time the expression for the scattering amplitude $f_k(\theta)$ in terms of phase shifts δ_l.

Finally, the differential scattering cross section is then given by

$$\left.\frac{d\sigma}{d\Omega}\right|_\theta = |f_k(\theta)|^2 = \frac{1}{k^2}\left|\sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)}e^{i\delta_l}\sin\delta_l\, Y_l^0(\theta)\right|^2 \tag{11.57}$$

from which we deduce the total scattering cross section by integrating over the angles

$$\begin{aligned}\sigma &= \int \left.\frac{d\sigma}{d\Omega}\right|_\theta d\Omega \\ &= \frac{1}{k^2}\sum_{l,l'} 4\pi \sqrt{(2l+1)(2l'+1)}e^{i(\delta_l-\delta_{l'})}\sin\delta_l\sin\delta_{l'}\int d\Omega\, Y_{l'}^{0*}(\theta)Y_l^0(\theta).\end{aligned} \tag{11.58}$$

Since spherical harmonics are orthonormal, we have

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \tag{11.59}$$

This result shows that the terms resulting from interference between waves of different angular momenta disappear from the total cross section. For any potential $V(r)$, the contribution $(2l+1)(4\pi/k^2)\sin^2\delta_l$ associated with a given value of l is positive and has an upper bound, for a given energy, of $(2l+1)(4\pi/k^2)$.

From the practical point of view, phase shift for each value of δ_l must be solved separately for each value of l (most of the time, moreover, this implies resorting to numerical techniques). In other words, the method of partial waves is attractive from a practical point of view only when there is a sufficiently small number of non-zero phase shifts.

For each value of the energy, there exists a critical value l_M of the angular momentum

$$\sqrt{l_M(l_M+1)} \simeq kr_0. \tag{11.60}$$

For local potentials, only the first few l values contribute.

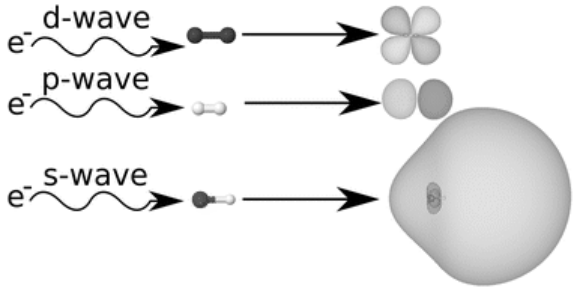


Figure 11.3: s, p, d wave scattering

For $l = 0$, we have s-wave scattering, here $\sigma(\theta) \sim \cos(\theta)$. For $l = 1$, we speak of p-wave scattering, and for $l = 2$, we have d-wave scattering. See s-, p- and d-wave scattering in Fig. 11.3

This allow us to solve inverse problem of identifying $V(\vec{r})$ from $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\big|_\theta$. When the potential $V(r)$ is unknown at the outset, we attempt to reproduce the experimental curves which give the differential cross section at a fixed energy by introducing a small number of non-zero phase shifts. Furthermore, the very form of the θ-dependence of the cross section often suggests the minimum number of phase shifts needed. For example, if we limit ourselves to the s-wave, the differential scattering cross section $\sigma(\theta)$ gives an isotropic differential cross section (Y_0^0 is a constant). If the experiments imply a variation of $\sigma(\theta)$ with θ, it means that phase shifts other than that of the s-wave are not equal to zero. Once we have thereby determined, from experimental results corresponding to different energies, the phase shifts which do effectively contribute to the cross section, we can look for theoretical models of potentials that produce these phase shifts and their energy dependence.

▪ **Exercise 11.1 — Properties of spherical Bessel functions.** Recall the definitions of the spherical Bessel and von Neumann functions (for $l \in \mathbb{N}$):

$$j_l(\rho) = (-1)^l \rho^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{\sin\rho}{\rho}, \tag{11.61}$$

$$y_l(\rho) = -(-1)^l \rho^l \left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\right)^l \frac{\cos\rho}{\rho}. \tag{11.62}$$

1. Compute the asymptotic behavior of j_l and y_l for $\rho \to 0$:

$$j_l(\rho) \sim \frac{\rho^l}{(2l+1)!!}, \tag{11.63}$$

$$y_l(\rho) \sim \frac{(2l-1)!!}{\rho^{l+1}}, \tag{11.64}$$

   "!!" is the double factorial, defined as $n!! = n \cdot (n-2) \cdot (n-4) \cdot \ldots$, with the usual convention $0!! = 1$.
2. Compute the asymptotic behavior of j_l and y_l for $\rho \to \infty$:

$$j_l(\rho) \sim \frac{1}{\rho} \sin\left(\rho - l\frac{\pi}{2}\right), \tag{11.65}$$

$$y_l(\rho) \sim \frac{1}{\rho} \cos\left(\rho - l\frac{\pi}{2}\right). \tag{11.66}$$

▪

▪ **Exercise 11.2 — Scattering phase shift in a Yukawa potential.** For a Yukawa potential,

$$V(r) = \frac{V_0}{\mu r} e^{-\mu r} \tag{11.67}$$

it can be shown that in the first Born approximation, the scattering amplitude is given by

$$f(\vec{p}' \leftarrow \vec{p}) = -\frac{2mV_0}{\mu} \frac{1}{2p^2(1-\cos\theta)+\mu^2} \tag{11.68}$$

θ is the angle between $\vec{p}$ and $\vec{p}'$, and $p = |\vec{p}| = |\vec{p}'|$; (we also consider $\hbar = 1$ as usual).

1. Obtain an expression for the scattering phase shift δ_l in terms of Legendre functions of the second kind:

$$Q_l(\zeta) = \frac{1}{2}\int_{-1}^{1} \frac{P_l(\zeta')}{\zeta - \zeta'} \mathrm{d}\zeta' \tag{11.69}$$

We will assume that $|\delta_l| \ll 1$.
Hint. Make use of the orthogonality of the Legendre polynomials:

$$\int_{-1}^{1} \mathrm{d}\zeta P_l(\zeta) P_{l'}(\zeta) = \frac{2\delta_{ll'}}{2l+1} \tag{11.70}$$

2. Use the expansion formula:

$$Q_l(\zeta) = \sum_{n=0}^{\infty} \frac{(l+2n)!}{(2l+2n+1)!!(2n)!!} \cdot \frac{1}{\zeta^{l+2n+1}} \tag{11.71}$$

to show the following:
   (a) δ_l is negative, resp. positive, when the potential is repulsive, resp. attractive.
   (b) When the de Broglie wavelength is much longer than the range of the potential, δ_l is proportional to p^{2l+1}. Find the proportionality constant.

▪

▪ **Exercise 11.3 — Scattering off a spherical potential.** Consider the potential $V(r)$ given by

$$V(r) = \begin{cases} 0 & \text{for } r > a, \\ \infty & \text{for } r < a. \end{cases} \tag{11.72}$$

1. Derive an expression for the s-wave $(l = 0)$ phase shift. (Refer to the detailed properties of the spherical Bessel functions to solve this problem).
2. What is the total cross section $\sigma = \int (\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}) \mathrm{d}\Omega$ in the extreme low-energy limit $k \to 0$? Compare your answer with the geometric cross section πa^2. Use the following relations:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2, \tag{11.73}$$

$$f(\theta) = \left(\frac{1}{k}\right) \sum_{l=0}^{\infty} (2l+1) e^{i\delta_l} \sin\delta_l P_l(\cos\theta). \tag{11.74}$$

▪

▪ **Exercise 11.4 — Scattering off a constant potential.** Consider a potential

$$V = \begin{cases} 0 & \text{for } r > R, \\ V_0 = \text{constant} & \text{for } r < R, \end{cases} \tag{11.75}$$

where V_0 may be positive or negative.

1. Using the method of partial waves, show that for $|V_0| \ll E = \frac{\hbar^2 k^2}{2m}$ and $kR \ll 1$, the differential cross section is isotropic and that the total cross section is given by

$$\sigma_{\text{tot}} = \left(\frac{16\pi}{9}\right)\left(\frac{m^2 V_0^2 R^6}{\hbar^4}\right). \tag{11.76}$$

2. Suppose the energy is raised slightly. Show that the angular distribution can then be written as

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = A + B\cos\theta. \tag{11.77}$$

Obtain an approximate expression for B/A.

▪

▪ **Exercise 11.5 — Scattering off a $\frac{1}{r^2}$ potential.** Let $(A > 0)$ and the potential

$$V(r) = \frac{\hbar^2 A}{2mr^2}. \tag{11.78}$$

1. Write down the eigenvalue equation of the Hamiltonian associated with this potential, and find a solution in terms of spherical Bessel functions.
2. Obtain the phase shifts exactly. Show that for $A \ll 1$, one approximately has

$$\delta_l = -\frac{\pi}{2}\frac{A}{2l+1}. \tag{11.79}$$

What is the value of the total cross section?

▪

IV Relativistic quantum mechanics

Lecture 12

> Motivation and failed attempts; Dirac equation; Pauli equation.

12.1 Motivation and failed attempts

So far our focus was on non-relativistic quantum physics. The latter is a well-established theory that provides us with an accurate description of diverse physical phenomena, including moving electrons in atoms, outcomes of many non-accelerator scattering experiments, radioactive decay etc. The applicability of the theory is, however, limited to small (compared to the speed of light) velocities of the constituents of a physical system. Hence, for example, in the cases when kinetic energies of particles involved in a scattering experiment become comparable with their rest energies, a new formalism must be adopted, which is consistent with the principles of special relativity. On the other hand, even in low-energy, low-velocity situations, relativistic corrections to the results obtained by solving the Schröedinger equation can give us an important information about the system; furthermore, these corrections can often be measured in experiment with a remarkable accuracy, as, for example, in the case of electron energy levels in atoms.

The framework that reconciles quantum postulates with the apparent Lorentz invariance of fundamental laws of Nature is called quantum field theory. In these notes, we do not aim to discuss quantum fields in any detail. Instead, in the remaining two lectures we outline the routes by which relativistic notions can be introduced in quantum mechanics without essential shifts of its "paradigms". Although limited in its depth, this approach allows us to look at certain results from a perspective that is missed when one derives them from the first principles of quantum field theory. That being said, we will largely follow the historical line of developments in the field, since the history of quantum fields, in fact, cannot be disentangled from the history of the "ordinary" quantum mechanics.[1] This will also enables us to see how heuristic (and, after all, not necessarily correct) arguments may lead to discoveries.

According to special relativity, physical laws are invariant under Lorentz transformations. For example, in going from one reference frame to another, moving with respect to the first one with the velocity v along the x-axis, one has

$$\begin{aligned} x \to x' &= \gamma\left[x - \frac{v}{c}(ct)\right] , \\ ct \to ct' &= \gamma\left[ct - \frac{v}{c}v\right] \end{aligned} \tag{12.1}$$

[1] See chapter 1 of [9] for an excellent historical introduction into quantum fields.

with $\gamma = \left(1 - v^2/c^2\right)^{-1}$. On the other hand, the cornerstone of the non-relativistic quantum mechanics — the Schrödinger equation

$$-\frac{\hbar}{i}\frac{\partial \psi}{\partial t} = H\psi \tag{12.2}$$

— is apparently not Lorentz invariant, since it contains the first derivative in time but the second derivative in space. Therefore, one should look for a Lorentz-invariant generalization of the Schrödinger equation, such that the latter is reproduced in the non-relativistic limit.[2] Below we first make two unsuccessful attempts for such a generalization and then, based on the gained experience, suggest the successful one.

1st failed attempt

The energy of a relativistic particle is given by

$$E = \sqrt{m^2c^4 + \boldsymbol{p}^2c^2}\,, \tag{12.3}$$

where m is the particle's mass, and $\boldsymbol{p}$ is its three-momentum. Let us apply the standard rules of quantum mechanics to the above relation and replace

$$\mathbf{p} \to \hat{\mathbf{p}} = -i\hbar\boldsymbol{\nabla}\,. \tag{12.4}$$

Then, the "relativistic Hamiltonian" in the x-representation reads

$$H = \sqrt{m^2c^4 - \hbar^2c^2\boldsymbol{\nabla}^2}\,, \tag{12.5}$$

and the Schrödinger equation becomes

$$-\frac{\hbar}{i}\frac{\partial \psi}{\partial t} = \sqrt{m^2c^4 - \hbar^2c^2\boldsymbol{\nabla}^2}\,\psi\,. \tag{12.6}$$

To reveal the problem with this equation, we rewrite its r.h.s. as

$$\sqrt{m^2c^4 - \hbar^2c^2\boldsymbol{\nabla}^2}\,\psi(x) = \int d^3\mathbf{x}' F(\mathbf{x},\mathbf{x}')\,\psi(\mathbf{x}') \tag{12.7}$$

with

$$F(\mathbf{x},\mathbf{x}') \propto \int d^3\mathbf{p}\, e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')}\,\sqrt{\mathbf{p}^2c^2 + m^2c^4}\,. \tag{12.8}$$

We conclude that the evolution of the wavefunction ψ at a given point $\mathbf{x}$ and at a given time t depends on the behaviour of ψ at the same moment of time t but at the points far away from $\mathbf{x}$. In other words, Eq. (12.6) violates causality. This contradicts the principles of special relativity according to which signals cannot propagate faster than the speed of light.

2nd failed attempt

Let us try to get rid of the unpleasant square root in Eq. (12.6) by taking squares of the operators on both sides:

$$\left(-\frac{\hbar}{i}\frac{\partial}{\partial t}\right)^2 \psi = \left(m^2c^4 - \hbar^2c^2\boldsymbol{\nabla}^2\right)\psi\,. \tag{12.9}$$

[2] This reasoning is not a bulletproof. One may argue that Eq. (12.2) is not *manifestly* Lorentz invariant, but it becomes so when written in a suitable form; cf. Maxwell's equations written in terms of spatial vectors or linearized Einstein's equations written in the harmonic gauge.

This equation is manifestly Lorentz invariant; it can be written as

$$-\Box\psi = \frac{m^2c^4}{\hbar^2}\psi\,, \tag{12.10}$$

where

$$\Box = \frac{\partial^2}{\partial t^2} - \boldsymbol{\nabla}^2 c^2 \tag{12.11}$$

is the d'Alambert operator. Eq. (12.10) is known as the Klein-Gordon equation. It is troubling for us for two reasons. First, notice that the time evolution of states with a definite momentum is determined by

$$\psi \sim e^{\frac{i}{\hbar}Et}\,, \quad E = \pm\sqrt{\mathbf{p}^2c^2 + m^2c^4}\,. \tag{12.12}$$

The states with both positive and negative energies are present. This means that the relativistic Hamiltonian is not bounded from below, and there is no ground state.[3] Second, in quantum physics the probability must conserve, and the probability density must be positive-definite:

$$\frac{d}{dt}\int d^3\mathbf{x}\,\psi^*\psi = 0\,, \quad \psi^*\psi \geqslant 0\,. \tag{12.13}$$

But this comes from the fact that ψ obeys the differential equation of the first order in time:

$$\frac{d}{dt}\int d^3\mathbf{x}\,\psi^*\psi = \int d^3\mathbf{x}\,(\dot\psi^*\psi + \psi^*\dot\psi) = \int d^3\mathbf{x}\left[(iH\psi)^*\psi - \psi^*(iH\psi)\right] = 0\,. \tag{12.14}$$

For the second-order in time equation like Eq. (12.10), this does not work. But, maybe, one should change the definition of probability density? The natural choice of a *conserved* quantity composed of ψ obeying Eq. (12.10) is

$$\rho = \frac{i}{2m}\left(\psi^*\frac{\partial}{\partial t}\psi - \psi\frac{\partial}{\partial t}\psi^*\right)\,. \tag{12.15}$$

This function is real, and

$$\frac{d}{dt}\int d^3\mathbf{x}\,\rho(\mathbf{x}) = 0\,. \tag{12.16}$$

Unfortunately, $\rho(\mathbf{x})$ is, in general, not positive-definite, and, hence, we cannot interpret it as a probability density.

12.2 The Dirac equation

Having learnt something from the considerations above, let us now look for a generalization of the Schrödinger equation, which would be of the first derivative in time and linear in momentum. The hope is that the first requirement will allow us to avoid the problem with negative probabilities, while the second requirement permits to treat space and time on equal footing, in accordance with special relativity. We keep the form (12.2) of the equation intact, and choose the Hamiltonian (in the momentum representation) as follows:

$$H = c\sum_{i=1}^{3}\alpha_i p_i + \beta mc^2\,. \tag{12.17}$$

[3] In classical physics and in the case $m > 0$ one can simply assume that the only physical states are those with positive energy. Because of the gap $2mc^2$, no continuous process can take a particle from positive to negative energy. In quantum physics this logic fails, since quantum transitions between different energy levels are possible.

With this expression, we try to reproduce the relativistic dispersion relation

$$H^2 = \mathbf{p}^2c^2 + m^2c^4 \,. \tag{12.18}$$

Taking square, one gets (we assume summation over repeating indices)

$$(c\alpha_i p_i + \beta mc^2)(c\alpha_j p_j + \beta mc^2) = c^2\alpha_i\alpha_j p_i p_j + mc^3(\beta\alpha_i + \alpha_i\beta)p_i + \beta^2 m^2c^4 \,. \tag{12.19}$$

Clearly, this is not equal to $p_i p_i c^2 + m^2c^4$ for any α_i, β c-numbers. Suppose then that they are not numbers but non-commuting matrices. The relation (12.18) is now satisfied if one demands

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij}, \quad \{\alpha_i, \beta\} = 0, \quad \beta^2 = 1 \,, \tag{12.20}$$

where we denoted $\{A, B\} \equiv AB + BA$. An additional requirement on the matrices α_i and β comes from the hermiticity of the Hamiltonian:

$$H^\dagger = H \quad \Rightarrow \quad \alpha_i^\dagger = \alpha_i \,, \;\; \beta^\dagger = \beta \,. \tag{12.21}$$

Let us have a closer look at $\boldsymbol{\alpha}$, β. The conditions (12.20) imply that they are all traceless. Indeed,

$$\mathrm{Tr}\,\alpha_i = \mathrm{Tr}\left(\alpha_i\beta^2\right) = \mathrm{Tr}\,(\beta\alpha_i\beta) = -\,\mathrm{Tr}\left(\alpha_i\beta^2\right) = -\,\mathrm{Tr}\,\alpha_i \quad \Rightarrow \quad \mathrm{Tr}\,\alpha_i = 0 \,, \tag{12.22}$$

$$\mathrm{Tr}\,\beta = \mathrm{Tr}\left(\beta\alpha_1^2\right) = \mathrm{Tr}\,(\alpha_1\beta\alpha_1) = -\,\mathrm{Tr}\left(\beta\alpha_1^2\right) = -\,\mathrm{Tr}\,\beta \quad \Rightarrow \quad \mathrm{Tr}\,\beta = 0 \,. \tag{12.23}$$

Next, from the fact that $\alpha_i^2 = \beta^2 = 1$ it follows that the eigenvalues of α_i and β are ± 1. Together with the tracelessness, this means that α_i and β must be even-dimensional square matrices. Consider first the 2×2 case. Any 2×2 matrix can be decomposed into a linear combination of the unit matrix I and the triplet of Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \,, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \,, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \,. \tag{12.24}$$

The Pauli matrices are traceless; there are, however, not enough of them to obtain the four linearly independent traceless matrices α_i, β. The 2×2 case is, therefore, discarded.

One can find the matrices obeying all the above requirements among 4×4 matrices. For example, the following choice works:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \,, \tag{12.25}$$

where I is the 2×2 unit matrix. This is known as the Dirac-Pauli representation of $\boldsymbol{\alpha}$, β. It is clear that the choice of the matrices is not unique; see Exercise 12.2 for more details. We can now write the famous Dirac equation

$$-\frac{\hbar}{i}\frac{\partial\psi_D}{\partial t} = H_D\psi_D \,, \quad H_D = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2 \,. \tag{12.26}$$

Since H_D is a 4×4 matrix, the Dirac wavefunction ψ_D is a four-component spinor. Hence, it describes four degrees of freedom. We will argue that two of them correspond to particle's spin, and the other two — to an antiparticle. It is easy to see that the Dirac equation possesses no problem with the probability density. Indeed, the latter is defined as $\psi_D^\dagger\psi_D$, and is positive-definite and conserved due to the hermiticity of H_D.

Let us study the eigenfunctions and eigenvalues of the Dirac Hamiltonian H_D:

$$H_D\psi = E\psi \,. \tag{12.27}$$

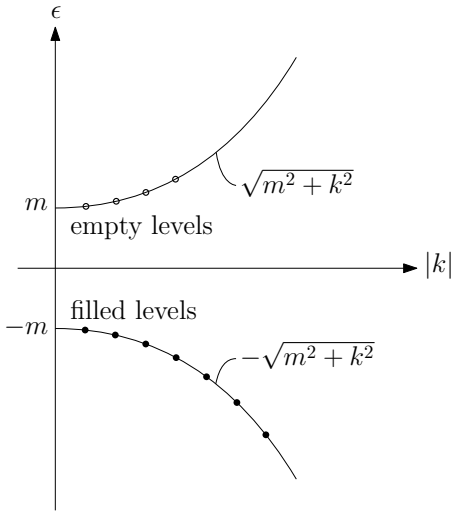


Figure 12.1: The Dirac sea of fermions.

Due to linearity, one can decompose ψ in Fourier modes. For a single Fourier harmonics, $\psi \sim e^{\frac{i}{\hbar}\mathbf{k}\cdot\mathbf{x}}$, the Dirac Hamiltonian becomes (we take, for simplicity, $\mathbf{k} = (0,0,k)^T$)

$$H_D = \begin{pmatrix} mc^2 & 0 & kc & 0 \\ 0 & mc^2 & 0 & -kc \\ kc & 0 & -mc^2 & 0 \\ 0 & -kc & 0 & -mc^2 \end{pmatrix} . \tag{12.28}$$

If we do the appropriate basis change to swap the second row with the third row and the second column with the third column, we get

$$H_D = \begin{pmatrix} H_1 & 0 \\ 0 & H_2 \end{pmatrix} , \quad H_1 = \begin{pmatrix} mc^2 & kc \\ kc & -mc^2 \end{pmatrix} , \quad H_2 = \begin{pmatrix} mc^2 & -kc \\ -kc & -mc^2 \end{pmatrix} . \tag{12.29}$$

The eigenvalues of H_1 and H_2 are, accordingly,

$$E_1 = +\sqrt{k^2c^2+m^2c^4}, \quad E_2 = -\sqrt{k^2c^2+m^2c^4} . \tag{12.30}$$

It appears that the problem of negative energies is still there. Dirac proposed a remarkable solution to this problem in 1930. It works provided that the physical system under consideration is composed of fermions obeying the Pauli exclusion principle (Dirac himself considered electrons). The system naturally seeks for the ground state. Dirac claimed the ground state to be that in which all negative energy levels are occupied by fermions (the "Dirac sea") and all positive energy levels are empty, see figure 12.1 for illustration. The exclusion principle prevents fermions from descending to ever decreasing energy levels, since all of them are full, hence such ground state is stable. Next, there can be two types of excitations above the ground state. One of them describes fermions occupying positive energy levels. Another type corresponds to the absence of a fermion at one of the negative energy levels. Such "hole" in the Dirac sea has a positive energy as compared to the ground state, but its quantum numbers are opposite to those of an "ordinary" fermion. For example, in the case of electrons, a hole has the electron mass but the positive electric charge. Dirac concluded that holes describe antiparticles. An antiparticle of the electron — the positron — was discovered by Anderson in 1932, and one year later Dirac got the Nobel prize.

The theory of Dirac had a great impact on the development of quantum physics. But it is not free from drawbacks. For example, the Dirac fermion must be a four-component spinor, unlike

certain fermions (named after Majorana) that are described just by two components. Also, being based on the Pauli exclusion principle, Dirac's argument seems to rule out the existence of any particles of integer spin, i.e., bosons. However, today we know a large amount of particles of zero spin (the elementary Higgs boson, or mesons composed of quark-antiquark pairs) as well as particles of spin one (the elementary gauge bosons). It is interesting to quote Julian Schwinger in this respect, who said: "The picture of an infinite sea of negative energy electrons is now best regarded as a historical curiosity, and forgotten." The truth is that, however, the Dirac's picture is now commonly used both in particle and solid-state physics (see Addendum A).

12.3 The Pauli equation

The Pauli equation describes a non-relativistic fermion in an external electromagnetic field. To derive it, we start with the relativistic Dirac equation (12.49) and make the replacement

$$p^\mu \;\Rightarrow\; \pi^\mu = p^\mu - \frac{e}{c}A^\mu \,, \quad \mu = 0,1,2,3 \,. \tag{12.31}$$

Here e is the electric charge and A^μ denotes the four-potential whose 0'th component is the scalar potential, $A^0 = \Phi$. The replacement (12.31) amounts to the substitution

$$-\frac{\hbar}{i}\frac{\partial}{\partial t} \to -\frac{\hbar}{i}\frac{\partial}{\partial t} - e\Phi \tag{12.32}$$

$$-i\boldsymbol{\nabla} \to -i\boldsymbol{\nabla} - \frac{e}{c}\mathbf{A} \,. \tag{12.33}$$

The Dirac equation becomes

$$-\frac{\hbar}{i}\frac{\partial \psi}{\partial t} = \left[c\boldsymbol{\alpha}\cdot\boldsymbol{\pi} + \beta mc^2 + e\Phi\right]\psi \,. \tag{12.34}$$

This equation allows us to determine, for example, energy levels of an electron in a static Coulomb field (for which $\mathbf{A} = 0$ and $\Phi = 1/r$) accounting for relativistic corrections.

We now want to solve Eq. (12.34) in the non-relativistic regime in which

$$pc \ll mc^2 \,, \quad e\Phi \ll mc^2 \,, \quad |e\mathbf{A}| \ll mc^2 \,. \tag{12.35}$$

It is convenient to use the two-component notation for the Dirac spinor:

$$\psi = \begin{pmatrix} \tilde{\phi} \\ \tilde{\chi} \end{pmatrix} \,, \tag{12.36}$$

where $\tilde{\phi}$ and $\tilde{\chi}$ are two-component spinors. Substitution to Eq. (12.34) gives

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\begin{pmatrix} \tilde{\phi} \\ \tilde{\chi} \end{pmatrix} = c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\begin{pmatrix} \tilde{\chi} \\ \tilde{\phi} \end{pmatrix} + e\Phi\begin{pmatrix} \tilde{\phi} \\ \tilde{\chi} \end{pmatrix} + mc^2\begin{pmatrix} \tilde{\phi} \\ -\tilde{\chi} \end{pmatrix} \,. \tag{12.37}$$

We use the following Ansatz to factor out the self-energy part:

$$\begin{pmatrix} \tilde{\phi} \\ \tilde{\chi} \end{pmatrix} = \exp\left(-\frac{imc^2}{\hbar}t\right)\begin{pmatrix} \phi \\ \chi \end{pmatrix} \,. \tag{12.38}$$

This yields

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\begin{pmatrix} \phi \\ \chi \end{pmatrix} = c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\begin{pmatrix} \chi \\ \phi \end{pmatrix} + e\Phi\begin{pmatrix} \phi \\ \chi \end{pmatrix} - 2mc^2\begin{pmatrix} 0 \\ \chi \end{pmatrix} \,, \tag{12.39}$$

or, in components,

$$-\frac{\hbar}{i}\frac{\partial\phi}{\partial t} = c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\chi + e\Phi\phi \tag{12.40}$$

$$-\frac{\hbar}{i}\frac{\partial\chi}{\partial t} = c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\phi + e\Phi\chi - 2mc^2\chi\ . \tag{12.41}$$

Let us analyze the second of the above equations. In the weak field limit, $e\Phi \ll 2mc^2$, we can drop out the term $e\Phi\chi$. This weak field approximation is valid when one deals, for example, with electrons in atoms. Indeed, the typical binding energy of the electron, ~ 13 eV, is much less than its rest energy $mc^2 \approx 5\cdot 10^5$ eV. Eq. (12.41) becomes

$$\chi = \frac{c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{2mc^2}\phi + \frac{\hbar}{i}\frac{1}{2mc^2}\frac{\partial\chi}{\partial t}\ . \tag{12.42}$$

This can be solved iteratively by assuming the last term in the r.h.s. to be small compared with other terms. The 0'th order approximation is written as

$$\chi^{(0)} = \frac{c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{2mc^2}\phi\ , \tag{12.43}$$

and the first order approximation is

$$\chi^{(1)} = \frac{c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{2mc^2}\phi + \frac{\hbar}{i}\frac{1}{2mc^2}\frac{\partial}{\partial t}\left(\frac{c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{2mc^2}\phi\right)\ . \tag{12.44}$$

We see that the second term in $\chi^{(1)}$ is indeed suppressed by an extra mc^2. We can, therefore, keep only the first term. Then, $\chi \ll \phi$, which justifies treating the term $\propto \partial\chi/\partial t$ as a small perturbation. χ is called the "small" component (of the Dirac spinor), and ϕ is called the "large" component. Inserting Eq. (12.43) into Eq. (12.40), we get

$$-\frac{\hbar}{i}\frac{\partial\phi}{\partial t} = \left(\frac{(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})}{2m} + e\Phi\right)\phi\ . \tag{12.45}$$

Now, we can use the fact that

$$(\boldsymbol{\sigma}\cdot\boldsymbol{a})(\boldsymbol{\sigma}\cdot\boldsymbol{b}) = \boldsymbol{a}\cdot\boldsymbol{b} + \boldsymbol{\sigma}\cdot(\boldsymbol{a}\times\boldsymbol{b}) \tag{12.46}$$

to transform the r.h.s. part of Eq. (12.45) (see Exercise 12.3):

$$(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}) = |\boldsymbol{\pi}|^2 + \boldsymbol{\sigma}\cdot(\boldsymbol{\pi}\times\boldsymbol{\pi}) = |\boldsymbol{\pi}|^2 - e\boldsymbol{\sigma}\cdot\mathbf{B}\ , \tag{12.47}$$

where the definition (12.31) of $\boldsymbol{\pi}$ was used. At last,

$$-\frac{\hbar}{i}\frac{\partial\phi}{\partial t} = \left[\frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 - \frac{e\hbar}{2mc}\boldsymbol{\sigma}\cdot\boldsymbol{B} + e\Phi\right]\phi\ , \tag{12.48}$$

and we have obtained the Pauli equation. The two components of the non-relativistic spinor ϕ correspond to two projections of its spin on a chosen axis.

Addendum A In particle physics, Dirac's picture of the "sea" of fermions occupying negative energy levels proved to be useful in studies, for example, of chiral anomaly and fermion number non-conservation in electroweak theory. In fact, the description of fermions and antifermions in terms of the Dirac sea and in terms of quantum fields are equivalent (see chapters 14-16 of [4]). For example, annihilation of a fermion and an antifermion corresponds to the transition of the particle from the positive energy level to the unoccupied negative energy level (figure 12.2(a)). The inverse transition from the negative to the positive energy level, caused, for example, by an external electromagnetic field, corresponds to the pair creation (figure 12.2(b)). Clearly, creating a particle-hole pair requires at least the energy of $2mc^2$, cf. Exercise 5.9. Note finally that the notion of particles and holes is also completely adequate in solid-state physics.

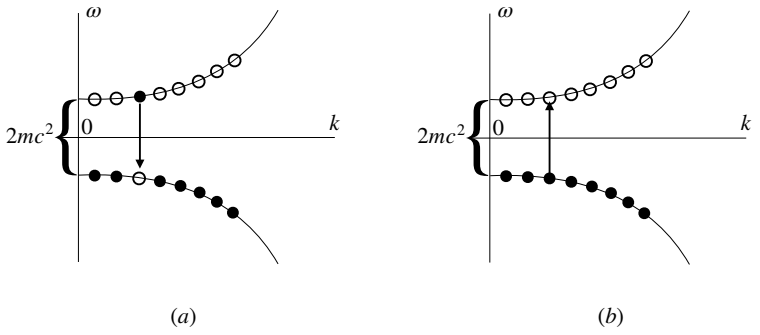


Figure 12.2: The Dirac sea picture of annihilation (a) and pair creation (b).

▪ **Exercise 12.1 — General solution of the Dirac equation.** Due to linearity, the Dirac equation

$$-\frac{\hbar}{i}\frac{\partial \Psi_D}{\partial t} = H_D \Psi_D \tag{12.49}$$

admits a decomposition of its general solution in terms of plane-wave functions,

$$\Psi_D = e^{\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x}-\omega_P t)} u_P \,, \tag{12.50}$$

where u_P is some function of the momentum $\mathbf{p}$.

1. Rewrite Eq. (12.49) as an equation on u_P.
2. Find the necessary and sufficient condition for this equation to have a non-zero solution. What is the physical meaning of this condition?
3. Find the general solution of the equation above.
   Hint: At this point it is convenient to remember that u_P is a column $(\phi_P,\ \chi_P)^T$ of two-component functions ϕ_P and χ_P.
4. Rewrite the general solution in the non-relativistic limit $p \ll mc$.

▪

▪ **Exercise 12.2 — Properties of the Dirac matrices.** Recall that the Dirac Hamiltonian H_D is given by the following 4×4 matrix,

$$H_D = \sum_{i=1}^{3} \alpha_i p_i + \beta m \,, \tag{12.51}$$

where

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} . \tag{12.52}$$

Here σ_i are the Pauli matrices, and I denotes the 2×2 identity matrix. The matrices α_i and β obey certain relations which, however, do not specify them fully, hence the choice (12.52) is not unique.

1. Given α_i, β, one can define new matrices α_i', β' via

   $$\alpha_i' = U\alpha_i U^{-1}, \quad \beta' = U\beta U^{-1}, \tag{12.53}$$

   where U is a unitary but otherwise arbitrary 4×4 matrix. Show that α_i', β' form an appropriate set of matrices provided that α_i, β do.
2. Find the matrix U that transforms β, given in Eq. (12.52), into $\beta' = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$. Find α_i' corresponding to this transformation. This choice of the Dirac matrices is called the Weyl representation.

3. Write the Dirac equation in the Weyl representation and in the notation $\Psi_D = (\phi,\ \chi)^T$. Take the limit $m = 0$, and check if the components ϕ and χ satisfy the Klein-Gordon equation. Find the solution of this equation for a massless particle propagating along the x-direction.
4. Find the representation of the Dirac matrices α', β' such that Im $\alpha'_i =$ Re $\beta' = 0$.

▪

▪ **Exercise 12.3 — One useful relation.** Show that

$$(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}) = |\boldsymbol{\pi}|^2 - \frac{e\hbar}{c}\boldsymbol{\sigma}\cdot\boldsymbol{B}\,, \tag{12.54}$$

where $\boldsymbol{\pi} = \boldsymbol{p} - \dfrac{e}{c}\boldsymbol{A}$, $\boldsymbol{B} = \text{rot}\,\boldsymbol{A}$, and $\boldsymbol{\sigma}$ denotes the triplet of the Pauli matrices.

▪

▪ **Exercise 12.4 — On Landau levels.** In this exercise we are interested in the energy levels of an electron in a uniform magnetic field. To find them, one should proceed in the same way as in the non-relativistic case. Namely, we take an *Ansatz* for stationary states,

$$\Psi = e^{-\frac{i}{\hbar}Et}\begin{pmatrix}\phi\\ \chi\end{pmatrix}\,, \tag{12.55}$$

and plug it into the Dirac equation in the external field, Eq. (12.34). This gives an eigenvalue problem for E whose solution will provide us with the desired energy levels.
Specifically, let us align the magnetic field along z-direction,

$$\boldsymbol{B} = \begin{pmatrix}0\\ 0\\ \mathscr{B}\end{pmatrix}\,. \tag{12.56}$$

We will work in the Dirac-Pauli representation of the matrices. For simplicity, we also put $\hbar = c = 1$.

1. Show that the magnetic field (12.56) is reproduced by the following combination of the potentials,

$$\boldsymbol{A} = -\begin{pmatrix}y\mathscr{B}\\ 0\\ 0\end{pmatrix}\,,\quad \Phi = 0\,. \tag{12.57}$$

   Is this choice of $\boldsymbol{A}$ and Φ unique?
2. Substituting the Ansatz (12.55) and the potentials (12.57) into Eq. (12.34), obtain an equation on the component ϕ.
3. Next, assume the following form of the general solution of the equation above,

$$\phi = e^{i(p_x x + p_z z)}\left(c_1\begin{pmatrix}F_+(y)\\ 0\end{pmatrix} + c_2\begin{pmatrix}0\\ F_-(y)\end{pmatrix}\right)\,, \tag{12.58}$$

   with c_1, c_2, p_x, p_z arbitrary constants. Find equations on the functions $F_+(y)$ and $F_-(y)$. By changing variables, reduce them to the form

$$\left(\frac{d^2}{d\xi^2} - \xi^2 + \alpha_\pm\right)F_\pm(\xi) = 0\,. \tag{12.59}$$

4. Eq. (12.59) is of Hermite's type. It admits solutions provided that $\alpha_\pm = 2n+1$, $n = 0,1,2,\ldots$. Having this in mind, derive the formula for the electron energy levels. What is the degeneracy of the ground level $n = 0$? Of the first excited level $n = 1$?

▪

Lecture 13

Relativistic corrections to the Pauli equation; relativistic description of bosons and fermions.

13.1 Relativistic corrections to the Pauli equation

The Pauli equation (12.48) can be rewritten in many useful ways, depending on a particular physical situation. Consider, for example, an electron moving in a weak external magnetic field,

$$\mathbf{B} = \mathrm{rot}\,\mathbf{A}\ , \quad \mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{r}\ . \tag{13.1}$$

Then, to the leading order in $\mathbf{A}$, the Pauli equation becomes

$$-\frac{\hbar}{i}\frac{\partial\phi}{\partial t} = \left[\frac{\mathbf{p}^2}{2m} - \mu(\mathbf{L}+2\mathbf{s})\cdot\mathbf{B}\right]\phi\ . \tag{13.2}$$

Here $\mathbf{L} = \mathbf{r}\times\mathbf{p}$ is the orbital momentum of the electron, $\mathbf{s} = \boldsymbol{\sigma}\hbar/2$ is its spin operator, and

$$\mu = \frac{e}{2mc} \tag{13.3}$$

is its magnetic moment. Note the factor 2 in front of $\mathbf{s}$ in the r.h.s. of the above equation, leading to the electron g-factor (the ratio of its magnetic to the mechanical moments) $g_e = 2$. The prediction of the correct value of g_e was the great success of the theory of Dirac.

Consider now an electron inside an atom, moving in a weak Coulomb field created by a nucleus of charge Z. Write the Pauli equation in the form

$$-\frac{\hbar}{i}\frac{\partial\phi}{\partial t} = \mathscr{H}_{\mathrm{Pauli}}\phi\ , \quad \mathscr{H}_{\mathrm{Pauli}} = \frac{\mathbf{p}^2}{2m} - \frac{Ze^2}{r}\ . \tag{13.4}$$

There is a systematic way to compute relativistic corrections to the Pauli Hamiltonian $\mathscr{H}_{\mathrm{Pauli}}$, which is based on the Foldy-Wouthuysen transformation. The first correction is of the order $(mc^2)^{-1}$. It reads as follows (see Exercise 13.1):

$$\mathscr{H}^{(1)} = \mathscr{H}_{\mathrm{Pauli}} + V_1 + V_2 + V_3\ . \tag{13.5}$$

Here

$$V_1 = -\frac{1}{2mc^2}\frac{\left(|\mathbf{p}|^2\right)^2}{4m^2} \tag{13.6}$$

is a relativistic correction to the kinetic energy of the electron,

$$V_2 = \frac{1}{2mc^2}\frac{1}{r}\frac{dV(r)}{dr}\mathbf{s}\cdot\mathbf{L}\,, \quad V(r) = -\frac{Ze^2}{r} \tag{13.7}$$

is the spin-orbit interaction of electron's spin with the Coulomb potential, and

$$V_3 = \frac{\hbar^2\pi}{2m^2c^2}Ze^2\delta(x) \tag{13.8}$$

is the so-called contact interaction (or the Darwin term). These relativistic corrections are used to determine the fine structure of energy levels of electrons. The latter were measured with a great accuracy for certain atoms (e.g., for a Hydrogen atom), allowing to test the predictions of relativistic quantum mechanics and quantum field theory.[1]

The perturbation theory with respect to c^{-1} is valid as long as

$$\frac{p^2}{2m} \ll m\,. \tag{13.9}$$

For an electron bound in the Coulomb potential created by a nucleus of charge Z, we have

$$\frac{p^2}{2m} \sim \frac{Ze^2}{r}\,. \tag{13.10}$$

Combining this with the uncertainty relation $pr \sim \hbar$ gives

$$p \sim \frac{mZe^2}{\hbar}\,, \tag{13.11}$$

which we can plug back into Eq. (13.9) to get

$$Z \ll \frac{1}{\alpha} \simeq 137\,, \tag{13.12}$$

where $\alpha = e^2/\hbar c$ is the fine-structure constant. We conclude that for heavy nuclei with $Z \gtrsim 137$ the perturbation theory is not applicable, and the treatment based on the exact Dirac equation is necessary. But, curiously, if one uses the Dirac equation with the Coulomb potential to compute electron energy levels in atoms with $Z \geqslant 137$, one finds that no stable electron orbits are possible. The physical meaning of this result is that heavy nuclei cannot be treated as point-like objects, and corrections to the Coulomb potential coming from the finite-size charge distribution of the nucleus must be taken into account.[2]

13.2 Relativistic description of bosons

In the previous lecture, we discussed various problems one encounters on the way of building the relativistic theory of quantum systems. Let us now outline a coherent framework in which these problems are overpassed. It was developed much in parallel with the developments in quantum mechanics. Historically, the first relativistic system which underwent quantization was the electromagnetic field. The corresponding particle — the photon — is a boson of spin one. Hence, we start in this section with the relativistic description of free bosons and, for simplicity, we neglect all its possible internal degrees of freedom.

[1] The accuracy in measuring the Hydrogen spectra is such that one needs to account for the finite size of the nucleus; in this case, the delta-function in the Darwin term must be replaced by a charge distribution inside the nucleus.

[2] See, e.g., §36 of [10].

A relativistic quantum system is necessarily a system of many particles. Imagine a collection of harmonic oscillators labelled by three real numbers $(k_x, k_y, k_z) = \mathbf{k}$, to be associated with the three-momentum of a particle. To each oscillator one can assign the creation and annihilation operators. The creation operator $a^\dagger(\mathbf{k})$ increases the number of particles in the $\mathbf{k}$'th oscillator by one. The annihilation operator $a(\mathbf{k})$ lowers this number by one. The operators obey the commutation relations

$$[a(\mathbf{k}), a(\mathbf{k}')] = 0\,, \quad [a^\dagger(\mathbf{k}), a^\dagger(\mathbf{k}')] = 0\,, \quad [a(\mathbf{k}), a^\dagger(\mathbf{k}')] = \delta(\mathbf{k}-\mathbf{k}')\,. \tag{13.13}$$

Next, we introduce the operator

$$\mathrm{H} = \int d^3\mathbf{k}\, \varepsilon_k\, a^\dagger(\mathbf{k}) a(\mathbf{k})\,, \quad \varepsilon_k = \sqrt{\mathbf{k}^2 + m^2} \tag{13.14}$$

called the Hamiltonian, and

$$\mathbf{P} = \int d^3\mathbf{k}\, \mathbf{k}\, a^\dagger(\mathbf{k}) a(\mathbf{k}) \tag{13.15}$$

called the momentum operator. By the means of these operators we want to investigate the structure of the Hilbert space $\mathscr{H}$ of the theory. Define the vacuum state $|0\rangle$ to be such that[3]

$$a(\mathbf{k})|0\rangle = 0 \quad \text{for any } \mathbf{k}\,. \tag{13.16}$$

If we act by $a^\dagger(\mathbf{k})$ on the vacuum state, we obtain the state $a^\dagger(\mathbf{k})|0\rangle$. Taking expectation values of H and $\mathbf{P}$ in this state give ε_k and $\mathbf{k}$ accordingly. We can interpret $a^\dagger(\mathbf{k})|0\rangle$ as a *one-particle* state, in which the particle has the energy ε_k and the momentum $\mathbf{k}$. By construction, the energy and the momentum obey the relativistic dispersion relation. Next, we can construct a *two-particle* state $a^\dagger(\mathbf{k}_1)a^\dagger(\mathbf{k}_2)|0\rangle$. The energy of this state, $\varepsilon_{k_1} + \varepsilon_{k_2}$ is the sum of the energies of the individual particles, and the momentum $\mathbf{k}_1 + \mathbf{k}_2$ is the sum of the individual momenta. This is how it should be in the free theory where particles do not interact. Acting further by $a^\dagger(\mathbf{k}_3)$ on a two-particle state, one obtains a three-particle state, and so on. The collection of the states

$$a^\dagger(\mathbf{k}_n)a^\dagger(\mathbf{k}_{n-1})\ldots a^\dagger(\mathbf{k}_2)a^\dagger(\mathbf{k}_1)|0\rangle \tag{13.17}$$

constitutes a basis in the Hilbert space $\mathscr{H}$ of the theory (the latter is called the Fock space). Hence, a general state $|\psi\rangle$ from $\mathscr{H}$ (a Fock state) admits a decomposition

$$|\psi\rangle = C_0\,|0\rangle + \int d^3\mathbf{k}\, C_1(\mathbf{k}) a^\dagger(\mathbf{k})\,|0\rangle + \int d^3\mathbf{k}_1 d^3\mathbf{k}_2\, C_2(\mathbf{k}_1,\mathbf{k}_2) a^\dagger(\mathbf{k}_1)a^\dagger(\mathbf{k}_2)\,|0\rangle + \ldots\,. \tag{13.18}$$

The theory we have just described does not suffer from any of the problems considered in the previous lecture. Indeed:

- the theory is relativistic,
- the energies of states of the theory are positive,
- the probability density is positive-definite, and the probability is conserved,
- the theory is causal and local; in fact, it coincides with the scalar field theory described by the Lagrangian density

$$L = \frac{1}{2}\dot{\varphi}^2 - \frac{1}{2}(\boldsymbol{\nabla}\varphi)^2 - \frac{1}{2}m^2\varphi^2\,. \tag{13.19}$$

[3] It is postulated that the vacuum state is unique.

Let us elaborate on the last item of the above list. Consider the theory of the free classical real scalar field φ with the Lagrangian density (13.19). One defines the momentum π as canonically conjugated to the variable φ:

$$\pi = \frac{\partial L}{\partial \dot{\varphi}} = \dot{\varphi} \,. \tag{13.20}$$

Next, one constructs the Hamiltonian density H:

$$H = \pi\dot{\varphi} - L = \frac{1}{2}\pi^2 + \frac{1}{2}(\boldsymbol{\nabla}\varphi)^2 + \frac{1}{2}m^2\varphi^2 \,, \tag{13.21}$$

so that the Hamiltonian is given by

$$\mathrm{H} = \int d^3\mathbf{x}\, H \,. \tag{13.22}$$

The canonical quantization procedure prescribes to treat the quantities φ, π as operators satisfying the commutation relations

$$[\varphi(\mathbf{x}), \varphi(\mathbf{y})] = 0 \,, \quad [\pi(\mathbf{x}), \pi(\mathbf{y})] = 0 \,, \quad [\varphi(\mathbf{x}), \pi(\mathbf{y})] = i\delta(\mathbf{x}-\mathbf{y}) \,. \tag{13.23}$$

Let us show that the resulting quantum theory is equivalent to the system of free bosons described above. To this end, we put the theory in a box of size L and decompose φ and π in Fourier modes:

$$\varphi(x) = \frac{1}{L^{3/2}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}\varphi(\mathbf{k}) \,, \quad \pi(x) = \frac{1}{L^{3/2}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}\pi(\mathbf{k}) \,. \tag{13.24}$$

In these expressions, the components k_x, k_y, k_z of $\mathbf{k}$ take the discrete set of values,

$$k_i = \frac{2\pi n_i}{L} \,, \quad i = x, y, z, \tag{13.25}$$

and the summation is performed over the integers n_x, n_y, n_z. If we now introduce the operators $a(\mathbf{k})$, $a^\dagger(\mathbf{k})$ according to

$$\begin{aligned} \varphi(\mathbf{k}) &= \frac{1}{\sqrt{2\varepsilon_k}}\left(a(\mathbf{k}) + a^\dagger(-\mathbf{k})\right) \\ i\pi(\mathbf{k}) &= \sqrt{\frac{\varepsilon_k}{2}}\left(a(\mathbf{k}) - a^\dagger(-\mathbf{k})\right) \end{aligned} \tag{13.26}$$

with $\varepsilon_k = \sqrt{\mathbf{k}^2 + m^2}$, we find that they satisfy the commutation relations (13.13). Furthermore, applying Eqs. (13.24) and (13.26) to Eq. (13.21), we get

$$\mathrm{H} = \sum_{\mathbf{k}} \varepsilon_k \left(a^\dagger(\mathbf{k})a(\mathbf{k}) + \frac{1}{2}\right) \,, \tag{13.27}$$

which coincides with Eq. (13.14) up to the vacuum energy contribution.

13.3 Relativistic description of fermions

The relativistic description of fermions is performed essentially in the same way as was done above for bosons; however, the relativistic framework must now accommodate the Pauli exclusion principle. To this end, the commutation relations for the creation and annihilation operators must be chosen in the following way:

$$\{a, a\} = 0 \,, \quad \left\{a^\dagger, a^\dagger\right\} = 0 \,, \quad \left\{a, a^\dagger\right\} = 1 \,. \tag{13.28}$$

Here $\{\cdot,\cdot\}$ denotes the anticommutator, and for simplicity we omit the arguments of the operators; they will be restored later. We want to make sure that with this definition, the occupation number of a fermionic state cannot exceed one. Consider the particle number operator

$$N_+ = a^\dagger a \,. \tag{13.29}$$

Let us first show that the eigenvalues $|\alpha\rangle$ of N_+ are real and non-negative. We have

$$a^\dagger a|\alpha\rangle = \alpha|\alpha\rangle \,, \tag{13.30}$$

hence,

$$\alpha = \langle\alpha|a^\dagger a|\alpha\rangle = \langle\alpha a|\alpha a\rangle \geqslant 0 \,. \tag{13.31}$$

Next, we want to show that α can only take values 0 or 1. The proof goes as follows:

$$\begin{aligned} a^2 = 0 \;\;\Rightarrow\;\; 0 = a^\dagger a a|\alpha\rangle &= (1 - aa^\dagger)a|\alpha\rangle \\ &= a|\alpha\rangle - a\alpha|\alpha\rangle = (1-\alpha)a|\alpha\rangle \,, \end{aligned} \tag{13.32}$$

and

$$\begin{aligned} (a^\dagger)^2 = 0 \;\;\Rightarrow\;\; a^\dagger a a^\dagger|\alpha\rangle &= a^\dagger(1 - a^\dagger a)|\alpha\rangle \\ &= a^\dagger(1-\alpha)|\alpha\rangle = a^\dagger|\alpha\rangle \,. \end{aligned} \tag{13.33}$$

We conclude that for a given eigenvalue $|\alpha\rangle$ the following is true:

$$\begin{aligned} &\text{either } \alpha = 1 \text{ or } a|\alpha\rangle = 0 \,, \\ &\text{either } \alpha = 0 \text{ or } a^\dagger|\alpha\rangle = 0 \,. \end{aligned} \tag{13.34}$$

Hence, the operators a, $a^\dagger$ act in a two-dimensional Hilbert space spanned by the eigenvectors of N_+. These are the states $|0\rangle$ and $|1\rangle$ such that

$$a|0\rangle = 0 \,, \quad a^\dagger|1\rangle = 0 \,. \tag{13.35}$$

Let us choose the state $|0\rangle$ to be the vacuum state (because of the symmetry between a and $a^\dagger$ expressed in Eqs. (13.35), this choice is a matter of convention). Then, $a^\dagger|0\rangle = |1\rangle$ is an excited state with the occupation number one. Thanks to the commutation relations (13.28), $a^2 = (a^\dagger)^2 = 0$. Hence, there are no states with occupation numbers larger than one. Thus, the Pauli exclusion principle is respected. If one defines the Hamiltonian according to

$$H = \omega a^\dagger a \,, \tag{13.36}$$

one obtains the energy of the vacuum state to be zero, and the energy of the excited state to be ω.

Since the operators a, $a^\dagger$ and N_+ act in a two-dimensional Hilbert space, they can be represented by 2×2 matrices:

$$a = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad a^\dagger = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad N_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \,. \tag{13.37}$$

In this representation, the eigenvectors of N_+ are

$$|0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \,. \tag{13.38}$$

Let us now account for the momentum $\mathbf{k}$ and spin σ of fermions. The generalization of the above construction is straightforward. The commutation relations (13.28) become

$$\{a_\sigma(\mathbf{k}), a_{\sigma'}(\mathbf{k}')\} = 0\,, \quad \{a_\sigma(\mathbf{k}), a^\dagger_{\sigma'}(\mathbf{k}')\} = \delta_{\sigma\sigma'}\delta(\mathbf{k}-\mathbf{k}')\,. \tag{13.39}$$

We would also like for our system to describes antifermions along with the fermions. To this end, introduce the creation $b^\dagger_\sigma(\mathbf{k})$ and annihilation $b_\sigma(\mathbf{k})$ operators of an antiparticle.[4] Their commutation relations are

$$\{b_\sigma(\mathbf{k}), b_{\sigma'}(\mathbf{k}')\} = 0\,, \quad \{b_\sigma(\mathbf{k}), b^\dagger_{\sigma'}(\mathbf{k}')\} = \delta_{\sigma\sigma'}\delta(\mathbf{k}-\mathbf{k}')\,, \tag{13.40}$$

and

$$\{a_\sigma(\mathbf{k}), b_{\sigma'}(\mathbf{k}')\} = 0\,, \quad \{a_\sigma(\mathbf{k}), b^\dagger_{\sigma'}(\mathbf{k}')\} = 0\,. \tag{13.41}$$

The vacuum state is defined as

$$a_\sigma(\mathbf{k})|0\rangle = b_\sigma(\mathbf{k})|0\rangle = 0 \;\text{ for any } \sigma,\, \mathbf{k}\,. \tag{13.42}$$

The Hamiltonian of the system reads as follows:

$$H = \sum_\sigma \int d^3\mathbf{k}\, \varepsilon_k \left[a^\dagger_\sigma(\mathbf{k}) a_\sigma(\mathbf{k}) + b^\dagger_\sigma(\mathbf{k}) b_\sigma(\mathbf{k})\right]\,, \quad \varepsilon_k = \sqrt{\mathbf{k}^2 + m^2}\,. \tag{13.43}$$

Finally, a general Fock state $|\psi\rangle$ of the Hilbert space is decomposed as

$$|\psi\rangle = C^{(0)}|0\rangle + \sum_\sigma \int d^3\mathbf{k}\, C^{(1)}_\sigma(\mathbf{k}) a^\dagger_\sigma(\mathbf{k})|0\rangle + \sum_\sigma \int d^3\mathbf{k}\, \tilde{C}^{(1)}_\sigma(\mathbf{k}) b^\dagger_\sigma(\mathbf{k})|0\rangle + \text{ many-particle states}\,. \tag{13.44}$$

The normalization of the Fock state implies

$$1 = |C^{(0)}|^2 + \sum_\sigma \int d^3\mathbf{k}\, |C^{(1)}_\sigma(\mathbf{k})|^2 + \sum_\sigma \int d^3\mathbf{k}\, |\tilde{C}^{(1)}_\sigma(\mathbf{k})|^2 + \ldots \tag{13.45}$$

The first term in this expansion determines the probability to have zero particles, the second term determines the probability to have one particle etc.

So far our discussion was limited to the free relativistic theories. In the real world, particles interact with each other, and processes involving creation and annihilation of different types of particles are possible. Consider, for example, the (free) neutron beta decay:

$$n \to p + e^- + \bar{\nu}_e\,. \tag{13.46}$$

Here n denotes neutron, p denotes proton, e^- stands for the electron (a β-particle), and $\bar{\nu}_e$ — for the electron antineutrino. The process (13.46) is described by the following part of the interaction Hamiltonian of the system:

$$H_{int} \sim G_F b^\dagger_{\nu_e} a^\dagger_e a^\dagger_p a_n\,. \tag{13.47}$$

Here G_F is Fermi's coupling constant. Its strength determines, in particular, the neutron mean lifetime τ. Experimentally $\tau \approx 14.69$ minutes.

[4] They are necessary to describe Dirac fermions. For Majorana fermions, a particle and an antiparticle are identical, and there is no need for another set of operators.

Note finally that, as in the case of bosons, one can construct a field theory whose quantization yields the free fermionic system described above. The Lagrangian density of the theory reads as follows:

$$L = \bar{\psi} i\gamma^\mu \partial_\mu \psi - m\bar{\psi}\psi\,, \quad \mu = 0,1,2,3. \tag{13.48}$$

Here ψ is the Dirac spinor, and the matrices γ^μ are related to the α_i and β matrices in the Dirac equation:

$$\beta = \gamma^0\,, \quad \alpha^i = \gamma^0\gamma^i\,. \tag{13.49}$$

▪ **Exercise 13.1 — Non-relativistic limit of the Dirac equation.** Previously we discussed the Dirac equation for a particle moving in an external electromagnetic field. Let us now investigate the non-relativistic limit of this equation which we expect to be of the form of the Schroedinger equation, and the form of the leading-order relativistic corrections. To simplify the treatment, consider the spherically-symmetric static electric field for which

$$\mathbf{A} = 0\,, \quad e\Phi = V(r)\,. \tag{13.50}$$

Then, the Dirac equation reads as follows,

$$H\Psi = \mathscr{E}\Psi\,, \quad H = c\boldsymbol{\alpha}\cdot\mathbf{p} + \beta mc^2 + V(r)\,, \quad \mathscr{E} = E + mc^2\,, \tag{13.51}$$

where $\Psi = (\phi,\ \chi)^T$ is the Dirac spinor and we put $\hbar = 1$. The non-relativistic limit implies

$$\frac{p^2}{2m} \ll mc^2\,, \quad V(r) \ll mc^2\,, \tag{13.52}$$

hence the expansion in Eq. (13.51) can be performed with respect to the speed of light c. We will work in the Dirac representation of the Dirac matrices.

1. Find the expression for χ through ϕ with the accuracy $\mathscr{O}(1/c^3)$. Using it, obtain an equation on ϕ with the accuracy $\mathscr{O}(1/c^2)$.
2. Rewrite the equation for ϕ in the form

   $$E\phi + \frac{p^2}{2m}\frac{E}{2mc^2}\phi = \tilde{H}\phi \tag{13.53}$$

   with $\tilde{H}$ some hermitian operator. To simplify the l.h.s. of Eq. (13.53), introduce a new variable

   $$\xi = \sqrt{1 + \frac{p^2}{2m}\frac{1}{2mc^2}}\,\phi \tag{13.54}$$

   and rewrite Eq. (13.53) in the form of the Schroedinger equation

   $$H_{eff}\xi = E\xi\,. \tag{13.55}$$

3. Extract the part of H_{eff} which does not depend on c. It should give you the usual Schroedinger equation on ξ.
4. Now extract the $\mathscr{O}(c^{-2})$-term in H_{eff} and bring it to the form

   $$\underbrace{-\frac{1}{2mc^2}\frac{(\mathbf{p}^2)^2}{4m^2}}_{\text{rel. correction to the energy}} + \underbrace{\frac{\hbar\boldsymbol{\sigma}}{2m\cdot 2mc^2}[\boldsymbol{\nabla}V, \mathbf{p}]}_{\text{spin-orbital interaction}} + \underbrace{\frac{\hbar^2}{8m^2c^2}\Delta V}_{\text{the Darwin term}}\,. \tag{13.56}$$

5. Rewrite the expression (13.56) for the Coulomb potential

$$V(r) = -\frac{Ze^2}{r} \,. \tag{13.57}$$

Indication: recall that the orbital momentum of the particle is $\mathbf{L} = \mathbf{x} \times \mathbf{p}$, and the vector of its spin is $\mathbf{s} = \hbar\boldsymbol{\sigma}/2$.

▪

▪ **Exercise 13.2 — Zitterbewegung.** The physical meaning of the first two relativistic corrections in Eq. (13.56) is quite clear: the first comes from the expansion of the relativistic energy of the particle, $E^2 = m^2c^4 + (p^2/2m)^2$, and the second represents the spin-orbital coupling. But what is the Darwin term? It can be attributed to a peculiar motion of a Dirac particle called *Zitterbewegung*. One way to see it is by using the Heisenberg equation of motion. Let us take the free particle Dirac Hamiltonian H_D, then

$$i\hbar\frac{d\mathscr{O}}{dt} = [\mathscr{O}, H_D] \,, \tag{13.58}$$

where $\mathscr{O}$ is some operator (an observable).

1. By taking $\mathscr{O} = \ddot{\boldsymbol{x}}$ in Eq. (13.58), obtain an equation on the observable $\dot{\boldsymbol{x}}$. Find the general solution of this equation. Integrating it, obtain an expression for the coordinate $\boldsymbol{x}$.
2. Determine all arbitrary constants in the expression for $\boldsymbol{x}$ found above by comparing its derivatives with the Heisenberg equations written for $\boldsymbol{x}$ and $\dot{\boldsymbol{x}}$.
3. What is the behavior of the coordinate $\boldsymbol{x}$? Does it oscillate and if so, what is the frequency of the oscillations (the formula for it and the numerical value)?
4. If the Dirac particle is moving in a (weak) external electric potential V, the average value of the potential felt by the particle is given by

$$\langle V \rangle = \frac{1}{2}\langle x^i x^j \rangle \frac{\partial^2 V}{\partial x^i \partial x^j} \,. \tag{13.59}$$

Making use of the explicit formula for $\boldsymbol{x}$, find $\langle V \rangle$. Compare with the third term of Eq. (13.56).
Hint: What is the value of $\langle x^i x^j \rangle$ in the isotropic background?

▪

▪ **Exercise 13.3 — Matrix mechanics of bosons.** Eqs. (13.37) determine an explicit matrix form of the fermionic creation and annihilation operators. In the case of bosons, the explicit form of the operators a and $a^\dagger$ can also be deduced. It was done by Born, Heisenberg and Jordan through their work on the harmonic oscillator.

1. Prove that a, $a^\dagger$ satisfying the commutation relations (13.13) cannot be finite dimensional matrices.
2. Find an explicit matrix representation of a and $a^\dagger$.

▪

Bibliography

[1] J.-P. Antoine, Quantum mechanics beyond hilbert space, in: A. Bohm, H.-D. Doebner, P. Kielanowski (Eds.), Irreversibility and Causality Semigroups and Rigged Hilbert Spaces, Springer Berlin Heidelberg, Berlin, Heidelberg, 1998, pp. 1–33.

[2] *NIST Digital Library of Mathematical Functions*, http://dlmf.nist.gov/, Release 1.0.20 of 2018-09-15, f. W. J. Olver, A. B. Olde Daalhuis, D. W. Lozier, B. I. Schneider, R. F. Boisvert, C. W. Clark, B. R. Miller and B. V. Saunders, eds.
URL http://dlmf.nist.gov/

[3] A. Andreassen, D. Farhi, W. Frost, M. D. Schwartz, Precision decay rate calculations in quantum field theory, Phys. Rev. D95 (8) (2017) 085011. arXiv:1604.06090, doi:10.1103/PhysRevD.95.085011.

[4] V. A. Rubakov, Classical theory of gauge fields, 2002.

[5] T. Marrodan Undagoitia, L. Rauch, Dark matter direct-detection experiments, J. Phys. G43 (1) (2016) 013001. arXiv:1509.08767, doi:10.1088/0954-3899/43/1/013001.

[6] B. Simon, Quantum Mechanics for Hamiltonians Defined as Quadratic Forms, Princeton Series in Physics, Princeton University Press, 2015.
URL https://books.google.ch/books?id=2259BgAAQBAJ

[7] J. Taylor, Scattering Theory: The Quantum Theory of Nonrelativistic Collisions, Dover Books on Engineering, Dover Publications, 2012.
URL https://books.google.ch/books?id=OIaXvuwZMLQC

[8] V. Vladimirov, A. Jeffrey, A. Littlewood, Equations of Mathematical Physics, Lecture notes in pure and applied mathematics, M. Dekker, 1971.
URL https://books.google.ch/books?id=oAfvAAAAIAAJ

[9] S. Weinberg, The Quantum theory of fields. Vol. 1: Foundations, Cambridge University Press, 2005.

[10] V. Berestetskii, L. Landau, E. Lifshitz, L. Pitaevskii, J. Sykes, Quantum Electrodynamics, Course of theoretical physics, Elsevier Science, 1982.
URL https://books.google.ch/books?id=URL5NKX8vbAC