Chapter 2. 1D Wave Mechanics

The main goal of this chapter is the solution and discussion of a few conceptually most important problems of wave mechanics for the simplest, 1D case. This lowest dimensionality, and a wide use of potential profiles’ approximation by sets of Dirac’s delta-functions, simplify the necessary calculations considerably without sacrificing the physical essence of the described phenomena. The reader is advised to pay special attention to Sections 6-9, which cover some important material not usually discussed in textbooks.

2.1. Probability current and uncertainty relations

As was discussed in the end of Chapter 1, in several cases (most importantly, at strong confinement within the \([y, z]\) plane), the general (3D) Schrödinger equation may be reduced to the 1D equation (1.92):

\[
\frac{i\hbar}{\partial t} \frac{\partial \Psi(x,t)}{\partial x} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + U(x,t)\Psi(x,t) .
\]  

(2.1)

If the transversal factor – say, the function \(YZ_1(y, z)\) that participates in Eq. (1.91), is normalized to unity, then the integration of Eq. (1.22a) over a segment \([x_1, x_2]\), gives the probability to find the particle on this segment:

\[
W(t) = \int_{x_1}^{x_2} \Psi(x, t)\overline{\Psi}(x, t) \, dx .
\]

(2.2)

If the particle under analysis is definitely inside the system, the normalization of its 1D wavefunction \(\Psi(x, t)\) is provided by extending integral (2) to the whole axis \(x\):

\[
\int_{-\infty}^{\infty} w(x, t) \, dx = 1, \quad \text{where} \quad w(x, t) = \Psi(x, t)\overline{\Psi}(x, t) .
\]

(2.3)

A similar integration of Eq. (1.23) shows that the expectation value of any operator depending only on coordinate \(x\) (and possibly time), may be expressed as

\[
\langle \mathcal{A} \rangle(t) = \int_{-\infty}^{\infty} \overline{\Psi}(x, t) \mathcal{A} \Psi(x, t) \, dx .
\]

(2.4)

It is also useful to introduce the probability current along the \(x\)-axis (a scalar):

\[
I(x, t) = \int j_x \, dy \, dz = \frac{\hbar}{m} \text{Im} \left( \overline{\Psi} \frac{\partial}{\partial x} \Psi \right) = \frac{\hbar}{m} \left| \Psi(x, t) \right|^2 \frac{\partial \phi}{\partial x} ,
\]

(2.5)

where \(j_x\) is \(x\)-component of the probability current density vector \(\mathbf{j}(r, t)\). Then the continuity equation (1.48) for the segment \([x_1, x_2]\) takes the form

\[
\frac{dW}{dt} + I(x_2) - I(x_1) = 0 .
\]

(2.6)

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The above formulas are the basis for the analysis of 1D problems of wave mechanics, but before proceeding to particular cases, let me deliver on my earlier promise to prove that Heisenberg’s uncertainty relation \(1.35\) is indeed valid for any wavefunction \(\Psi(x,t)\). For that, let us consider an evidently positive (or at least non-negative) integral

\[
J(\lambda) \equiv \int_{-\infty}^{\infty} \left| x\Psi + \lambda \frac{\partial \Psi}{\partial x} \right|^2 \; dx \geq 0, 
\]  

(2.7)

where \(\lambda\) is an arbitrary real constant, and assume that at the at \(x \rightarrow \pm \infty\) the wavefunction vanishes, together with its first derivative. The left-hand part of Eq. (7) may be recast as

\[
\int_{-\infty}^{\infty} x\Psi \Psi^* \; dx + \lambda \int_{-\infty}^{\infty} \left( \Psi \frac{\partial \Psi^*}{\partial x} + \frac{\partial \Psi}{\partial x} \Psi^* \right) \; dx + \lambda^2 \int_{-\infty}^{\infty} \frac{\partial \Psi}{\partial x} \frac{\partial \Psi^*}{\partial x} \; dx.
\]

(2.8)

According to Eq. (4), the first term in the last form of Eq. (8) is just \(\langle x^2 \rangle\). The second and the third integrals may be worked out by parts:

\[
\int_{-\infty}^{\infty} x\Psi \Psi^* \; dx = \int_{-\infty}^{\infty} x \frac{\partial}{\partial x} (\Psi \Psi^*) \; dx = \left[ x\Psi \Psi^* \right]_{x=-\infty}^{x=\infty} - \int_{-\infty}^{\infty} \Psi \Psi^* \; dx = -1, \quad (2.9)
\]

\[
\int_{-\infty}^{\infty} \frac{\partial \Psi}{\partial x} \frac{\partial \Psi^*}{\partial x} \; dx = \int_{-\infty}^{\infty} \frac{\partial \Psi}{\partial x} \Psi^* \; dx \bigg|_{x=+\infty} - \Psi \Psi^* \bigg|_{x=-\infty} + \int_{-\infty}^{\infty} \Psi^* \frac{\partial^2 \Psi}{\partial x^2} \; dx = \frac{1}{\hbar^2} \int_{-\infty}^{\infty} \Psi^* \hat{p}_x^2 \Psi \; dx = \frac{\langle p_x^2 \rangle}{\hbar^2}. \quad (2.10)
\]

As a result, Eq. (7) takes the following form:

\[
J(\lambda) = \langle x^2 \rangle - \lambda + \frac{\lambda^2 \langle p_x^2 \rangle}{\hbar^2} \geq 0, \quad \text{i.e. } \lambda^2 + a\lambda + b \geq 0, \quad \text{with } a = -\frac{\hbar^2}{\langle p_x^2 \rangle} \text{ and } b = \frac{\hbar^2 \langle x^2 \rangle}{\langle p_x^2 \rangle}. \quad (2.11)
\]

This inequality should be valid for any real \(\lambda\), i.e. the corresponding quadratic equation, \(\lambda^2 + a\lambda + b = 0\), can have either one (degenerate) real root - or no real roots at all. This is only possible if its determinant, \(\text{Det} = a^2 - 4b\), is non-positive, leading to the following requirement:

\[
\langle x^2 \rangle \langle p_x^2 \rangle \geq \frac{\hbar^2}{4}. \quad (2.12)
\]

In particular, if \(\langle x \rangle = 0\) and \(\langle p_x \rangle = 0\), then according to Eq. (1.33), Eq. (12) takes the form

\[
\langle x^2 \rangle \langle p_x^2 \rangle \geq \frac{\hbar^2}{4}, \quad (2.13)
\]

which, according to the definition (1.34) of r.m.s. uncertainties, is equivalent to Eq. (1.35).

\[1\] Eq. (13) may be proved even if \(\langle x \rangle\) and \(\langle p_x \rangle\) are not equal to zero, by making the following replacements, \(x \rightarrow x - \langle x \rangle, \partial/\partial x \rightarrow \partial/\partial \hat{x} + i\hat{p}/\hbar\), in Eq. (7), and then repeating all the calculations – which become rather bulky. We will re-derive the uncertainty relations, in a more efficient way, in Chapter 4.
Now let us notice that the Heisenberg’s uncertainty relation looks very similar to the commutation relation between the corresponding operators:

$$\left[\hat{x}, \hat{p}_x\right] \Psi := \left(\hat{x}\hat{p}_x - \hat{p}_x\hat{x}\right)\Psi = -i\hbar x \frac{\partial \Psi}{\partial x} + i\hbar \frac{\partial}{\partial x} \left(x\Psi\right) = i\hbar \Psi.$$  \hspace{1cm} (2.14a)

Since this relation is valid for arbitrary wavefunction $\Psi(x, t)$, we may present it as an operator equality:

$$\left[\hat{x}, \hat{p}_x\right] = i\hbar \neq 0.$$ \hspace{1cm} (2.14b)

In Sec. 4.5 we will see that the relation between Eqs. (13) and (14) is just a particular case of a general relation between the expectation values of non-commuting operators and their commutators.

### 2.2. Free particle: Wave packets

Let us start our discussion of particular problems with free the 1D motion, with $U(x, t) = 0$. From our discussion of Eq. (1.29) in Chapter 1, it is clear that in the 1D case, a similar “fundamental” (i.e. a particular but the most important) solution of the Schrödinger equation (1) is a monochromatic wave

$$\Psi_0(x, t) = \text{const} \times e^{i(k_0 x - \omega_0 t)}.$$ \hspace{1cm} (2.15)

According to Eqs. (1.32), it corresponds to a particle with an exactly defined momentum $^2 p_0 = \hbar k_0$ and energy $E_0 = \hbar \omega_0 = \hbar^2 k_0^2/2m$. However, for this wavefunction, product $\Psi^*\Psi$ does not depend on either $x$ or $t$, so that the particle is completely delocalized, i.e. its probability is spread all over axis $x$, at all times. (As a result, such state is still compatible with Heisenberg’s uncertainty relation (13), despite the exact value $p_0$ of momentum $p$.)

In order to describe a space-localized particle, let us form, at the initial moment of time ($t = 0$), a wave packet of the type shown in Fig. 1.6, by multiplying the sinusoidal waveform (15) by some smooth envelope function $A(x)$. As the most important particular example, consider a Gaussian packet

$$\Psi(x, 0) = A(x) e^{ik_0 x}, \quad \text{with} \quad A(x) = \frac{1}{(2\pi)^{1/4} (\delta x)^{1/2}} \exp\left\{-\frac{x^2}{2(\delta x)^2}\right\}.$$ \hspace{1cm} (2.16)

(By the way, Fig. 1.6 shows exactly such a packet.) The pre-exponential factor in this envelope function has been selected in the way to have the initial probability density,

$$w(x, 0) = \Psi^* (x, 0)\Psi(x, 0) = A^* (x)A(x) = \frac{1}{(2\pi)^{1/2} \delta x} \exp\left\{-\frac{x^2}{2(\delta x)^2}\right\},$$ \hspace{1cm} (2.17)

normalized according to Eq. (3), for any parameters $\delta x$ and $k_0$.\(^3\)

In order to explore the evolution of this packet in time, we could try to solve Eq. (1) with the initial condition (16) directly, but in the spirit of the discussion in Sec. 1.5, it is easier to proceed

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\(^2\) From this point on, in this chapter I will drop index $x$ in notation for $x$-component of vectors $\mathbf{k}$ and $\mathbf{p}$.

\(^3\) This may be readily proven using the well-known integral of the Gaussian function (“bell curve”) given by Eq. (17) – see, e.g., MA Eq. (6.9b). It is also straightforward to use MA Eq. (6.9c) to prove that for wave packet (16), parameter $\delta x$ is indeed the r.m.s. uncertainty (1.34) of coordinate $x$, thus justifying its notation.
differently. Let us first present the initial wavefunction \((16)\) as a sum \((1.65)\) of eigenfunctions \(\psi_k(x)\) of the corresponding stationary 1D Schrödinger equation \((1.60)\), in our current case

\[
-\frac{\hbar^2}{2m} \frac{d^2\psi_k}{dx^2} = E_k \psi_k, \quad \text{with} \quad E_k = \frac{\hbar^2 k^2}{2m},
\]

that are simply monochromatic waves,

\[
\psi_k = a_k e^{ikx},
\]

with a continuum spectrum of possible wave numbers \(k\). For that, sum \((1.65)\) should be replaced with an integral:

\[
\Psi(x,0) = \int a_k \psi_k(x) dx = \int a_k e^{ikx} dk.
\]

Now let us notice that from the point of view of mathematics, Eq. \((20)\) is just the usual Fourier transform from variable \(k\) to the “conjugate” variable \(x\), and we can use the well-known formula of the reciprocal Fourier transform to calculate

\[
a_k = \frac{1}{2\pi} \int \Psi(x,0) e^{-ikx} dx = \frac{1}{2\pi} \frac{1}{(\Delta x)^{1/2}} \int \exp \left\{ -\frac{x^2}{(2\Delta x)^2} - ikx \right\} dx, \quad \text{where} \quad \tilde{k} = k - k_0, \quad (2.21)
\]

This **Gaussian integral** may be worked out by the following standard method. Let us complement the exponent to the full square of a linear combination of \(x\) and \(k\), plus a term independent of \(x\):

\[
-\frac{x^2}{(2\Delta x)^2} - ikx = -\frac{1}{(2\Delta x)^2} \left[ x + 2i\tilde{k}(\Delta x)^2 \right]^2
\]

Since the integration in the right-hand part of Eq. \((20)\) should be performed at constant \(\tilde{k}\), in the infinite limits, its result would not change if we replace \(dx\) by \(dx' = d[x + 2i(\Delta x)^2 \tilde{k}]\).\(^5\) As a result, we get,

\[
a_k = \frac{1}{2\pi} \frac{1}{(\Delta x)^{1/2}} \int \exp \left\{ -\tilde{k}^2(\Delta x)^2 \right\} dx' = \left( \frac{1}{2\pi} \right)^{1/2} \frac{1}{(\Delta x)^{1/2}} \int \exp \left\{ -\tilde{k}^2(2\Delta x)^2 \right\}.
\]

so that \(a_k\) also has a Gaussian distribution, now along axis \(k\), centered to value \(k_0\) (Fig. 1.6b), with constant \(\Delta k\) defined as

\[
\Delta k = 1/2\Delta x.
\]

Thus we may present the initial wave packet \((16)\) as

\[
\Psi(x,0) = \left( \frac{1}{2\pi} \right)^{1/2} \frac{1}{(2\pi)^{1/4}(\Delta k)^{1/2}} \int \exp \left\{ -\frac{(k-k_0)^2}{(2\Delta k)^2} \right\} e^{ikx} dk.
\]

From comparison of this formula with Eq. \((16)\), it is evident that the r.m.s. uncertainty of the wave number \(k\) in this packet is indeed equal to \(\Delta k\) defined by Eq. \((24)\), thus justifying the notation.

\(^4\) For notation’s brevity, from this point on the infinite limit signs will be dropped in all 1D integrals.

\(^5\) The fact that the argument shift is imaginary is not important, because function under the integral is analytical, and tends to zero at Re \(x'\) → ±∞.
comparison of that relation with Eq. (1.35) shows that the Gaussian packet presents the ultimate case in
which the product $\Delta x \Delta p = \Delta x (\hbar \Delta k)$ has the lowest possible value ($\hbar/2$); for any other envelope’s shape the
uncertainty product may only be larger. We could of course get the same result for $\Delta k$ from Eq. (16)
using definitions (1.23), (1.33), and (1.34); the real advantage of Eq. (24) is that it can be readily
generalized to $t > 0$.

Indeed, we already know that the time evolution of the wavefunction is given by Eq. (1.67), for
our case giving$^6$

$$
\Psi(x,t) = \left(\frac{1}{2\pi}\right)^{1/2} \frac{1}{(2\pi)^{1/4}(\Delta k)^{1/2}} \int \exp\left\{ -\frac{(k - k_0)^2}{(2\Delta k)^2} \right\} e^{ikx} \exp\left\{ -im\frac{\hbar k^2}{2m} - i\frac{\hbar k^2}{2m} - \frac{\hbar k^2}{2m} \right\} dk.
$$

(2.26)

Fig. 1 shows several snapshots of the real part of wavefunction (26), for a particular case $\Delta k = 0.1 k_0$.

The plots clearly show the following effects:

(i) the wave packet as a whole (as characterized by its envelope) moves along the $x$ axis with a
certain group velocity $v_{gr}$.

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$^6$ Note that this packet is equivalent to Eq. (16) and hence is properly normalized to 1 – see Eq. (3). Hence the
wave packet introduction offers a natural solution to the problem of infinite wave normalization, which was
mentioned in Sec. 1.2.
(ii) the “carrier” wave inside the packet moves with a different, phase velocity \(v_{\text{ph}}\), which may be defined as the velocity the spatial points where wave’s phase \(\varphi(x, t) \equiv \arg \Psi\) takes a certain fixed value (say, \(\varphi = \pi/2\), where \(\text{Re} \Psi\) vanishes), and

(iii) the packet’s spatial width gradually increases with time - the packet spreads.

All these effects are common for waves of any physical nature. 7 Indeed, let us consider a 1D wave packet of the type (26),

\[
\Psi(x, t) = \int a_k e^{i(kx-\omega t)} \, dk ,
\]

propagating in a media with an arbitrary (but smooth!) dispersion relation \(\omega(k)\), and assume that the wave number distribution \(a_k\) is arbitrary but narrow: \(\delta k \ll \langle k \rangle = k_0\) - see Fig. 1.6b. Then we may expand function \(\omega(k)\) into the Taylor series near the central point \(k_0\), and keep only two of its leading terms:

\[
\omega(k) \approx \omega_0 + \frac{d\omega}{dk} \tilde{k} + \frac{1}{2} \frac{d^2\omega}{dk^2} \tilde{k}^2 , \quad \text{where } \tilde{k} \equiv k - k_0 , \quad \omega_0 \equiv \omega(k_0) , \quad (2.28)
\]

and both derivatives are also evaluated at point \(k = k_0\). In this approximation, 8 the expression in parentheses in the right-hand part of Eq. (27) may be rewritten as

\[
kx - \omega t = k_0 x + \tilde{k} x - \left( \omega_0 + \frac{d\omega}{dk} \tilde{k} + \frac{1}{2} \frac{d^2\omega}{dk^2} \tilde{k}^2 \right) t = \left( k_0 x - \omega_0 t \right) + \tilde{k} \left( x - \frac{d\omega}{dk} t \right) - \frac{1}{2} \frac{d^2\omega}{dk^2} \tilde{k}^2 t , \quad (2.29)
\]

so that Eq. (27) is reduced to integral

\[
\Psi(x, t) = e^{i(k_0 x - \omega_0 t)} \int a_k \exp \left[ i \left( \tilde{k} \left( x - \frac{d\omega}{dk} t \right) - \frac{1}{2} \frac{d^2\omega}{dk^2} \tilde{k}^2 t \right) \right] \, d\tilde{k} . \quad (2.30)
\]

First, let neglect the last term in square brackets (which is much smaller than the first term if the dispersion relation is smooth enough and/or the time interval \(t\) is sufficiently small), and compare the result with the initial form of the wave packet (27)

\[
\Psi(x, 0) = \int a_k e^{ikx} \, dk = A(x) e^{ik_0 x} , \quad \text{with } A(x) \equiv \int a_k e^{ikx} \, dk . \quad (2.31)
\]

The comparison shows that Eq. (30) is reduced to

\[
\Psi(x, t) = A(x - v_{\text{gr}} t) e^{ik_0(x-v_{\text{ph}} t)} , \quad (2.32)
\]

where \(v_{\text{gr}}\) and \(v_{\text{ph}}\) are two constants with the dimension of velocity:

\[
v_{\text{gr}} \equiv \frac{d\omega}{dk} \bigg|_{k=k_0} , \quad \text{and } v_{\text{ph}} \equiv \frac{\omega}{k} \bigg|_{k=k_0} . \quad (2.33)
\]

It is clear that Eq. (32) describes effects (i) and (ii) listed above. Let us calculate the group and phase velocities for the particular case of de Broglie waves whose dispersion law is given by Eq. (1.30):

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7 See, e.g., brief discussions in CM Sec. 5.3 and EM Sec. 7.2.
8 By the way, in the particular case of de Broglie wave described by dispersion relation (1.30), Eq. (28) is exact, because \(\omega = E/\hbar\) is a quadratic function of \(k = p/\hbar\), and all higher derivatives of \(\omega\) over \(k\) vanish for any \(k_0\).
\[ \omega = \frac{\hbar k^2}{2m}, \quad v_{\text{gr}} \equiv \frac{d\omega}{dk}\bigg|_{k=k_0} = \frac{\hbar k_0}{m} \equiv v_0, \quad v_{\text{ph}} \equiv \frac{\omega}{k}\bigg|_{k=k_0} = \frac{\hbar k_0}{2m} = \frac{v_{\text{gr}}}{2}. \quad (2.34) \]

We see that (very fortunately!) the velocity of the wave packet envelope is constant and equals to that of the classical particle moving by inertia, in accordance with the correspondence principle.

The remaining term in the square brackets of Eq. (30) describes effect (iii), the wave packet’s spread. It may be readily evaluated if the packet (27) is initially Gaussian, as in our example (25):

\[ a_k = \text{const} \times \exp\left\{ -\frac{\tilde{k}^2}{(2\delta k)^2} \right\}. \quad (2.34) \]

In this case integral (30) is Gaussian, and may be worked out exactly as integral (20), i.e. merging the exponents under the integral, and presenting them as a full square of linear combination of \( x \) and \( k \):

\[ -\frac{\tilde{k}^2}{(2\delta k)^2} + i\tilde{k}(x-v_{\text{gr}}t) - \frac{i}{2} \frac{d^2\omega}{dk^2} \tilde{k}^2 t = -\Delta(t)\left( \tilde{k} + i\frac{x-v_{\text{gr}}t}{2\Delta(t)} \right)^2 - \frac{(x-v_{\text{gr}}t)^2}{4\Delta(t)} + ik_0x - \frac{i}{2} \frac{d^2\omega}{dk^2} k_0^2 t, \quad (2.35) \]

where I have introduced the following complex function of time:

\[ \Delta(t) = \frac{1}{4(\delta k)^2} + \frac{i}{2} \frac{d^2\omega}{dk^2} t = (\delta x)^2 + \frac{i}{2} \frac{d^2\omega}{dk^2} t, \quad (2.36) \]

and have used Eq. (24) in the second equality. Now integrating over \( \tilde{k} \), we get

\[ \Psi(x,t) \propto \exp\left\{ -\frac{(x-v_{\text{gr}}t)^2}{4\Delta(t)} + i\left( k_0x - \frac{1}{2} \frac{d^2\omega}{dk^2} k_0^2 t \right) \right\}. \quad (2.37) \]

The imaginary part of ratio \( 1/\Delta(t) \) in the exponent gives just an additional contribution to wave’s phase, and does not affect the resulting probability distribution

\[ w(x,t) = \Psi^*\Psi \propto \exp\left\{ -\frac{(x-v_{\text{gr}}t)^2}{2\Delta(t)} \right\} \]

This is again a Gaussian bell curve spread over axis \( x \), centered to point \( \langle x \rangle = v_{\text{gr}}t \), with the r.m.s. width

\[ (\delta x')^2 \equiv \left\{ \frac{\text{Re}\left[ \frac{1}{\Delta(t)} \right]}{(\delta x)^2} \right\}^{-1} = (\delta x)^2 + \left( \frac{1}{2} \frac{d^2\omega}{dk^2} t \right)^2 \frac{1}{(\delta x)^2}. \quad (2.39a) \]

In the particular case of de Broglie waves, \( d^2\omega/dk^2 = \hbar/m \), so that

\[ (\delta x')^2 = (\delta x)^2 + \left( \frac{\hbar t}{2m} \right)^2 \frac{1}{(\delta x)^2}. \quad (2.39b) \]

The physics of the spreading is very simple: if \( d^2\omega/dk^2 \neq 0 \), the group velocity \( d\omega/dk \) of each small group \( dk \) of monochromatic components of the wave packet is different, resulting in the gradual (eventually, linear) accumulation of the differences of the distances traveled by the groups. The most curious feature of Eq. (39) is that the packet width at \( t > 0 \) depends on its initial width \( \delta x'(0) = \delta x \) in a
non-monotonic way, tending to infinity at both $\delta x \to 0$ and $\delta x \to \infty$. Because of that, for a fixed $t$, there is an optimal value of $\delta x$ with minimizes $\delta x'$:

$$\left(\delta x'\right)_{\text{min}} = \sqrt{2} \left(\delta x\right)_{\text{opt}} = \left(\frac{ht}{m}\right)^{1/2}. \quad (2.40)$$

This expression may be used for spreading effect estimates. Due to the smallness of the Planck constant $\hbar$ on the human scale of things, for macroscopic bodies this effect is extremely small even for very long time intervals; however, for light particles it may be very noticeable: for the electron ($m = m_e \approx 10^{-30}$ kg), and $t = 1$ s, Eq. (40) yields $(\delta x')_{\text{min}} \sim 1$ cm!

Note also that for any $t \neq 0$, the wave packet retains its Gaussian envelope, but the ultimate relation (24) is not satisfied, $\delta x' \delta p > \hbar/2$ - due to a gradually accumulated phase shift between the component monochromatic waves. The last remark on this topic: in quantum mechanics, the wave packet spreading is not an ubiquitous effect! For example, in Chapter 5 we will see that in a quantum oscillator, the spatial width of a Gaussian packet (for that system, called the Glauber state) does not grow monotonically but rather stays constant or oscillates in time.

Now let us briefly discuss the case when the initial wave packet is not Gaussian, but is described by an arbitrary initial wavefunction. In order to make the forthcoming result more appealing, it is beneficial to generalize out calculations to an arbitrary initial time $t_0$; it is evident that if $U$ does not depend on time explicitly, it is sufficient to replace $t$ with $(t - t_0)$ in all above formulas. With this replacement, Eq. (27) becomes

$$\Psi(x,t) = \int a_k e^{i[kx - \omega(t - t_0)]} dk, \quad (2.41)$$

and the reciprocal transform (21) reads

$$a_k = \frac{1}{2\pi} \int \Psi(x,t_0) e^{-ikx} dx. \quad (2.42)$$

If we want to express these two formulas with one relation, i.e. plug Eq. (42) into Eq. (41), we should give the integration variable $x$ some other name, e.g., $x_0$. The result is

$$\Psi(x,t) = \frac{1}{2\pi} \int dk \left[ \int dx_0 \Psi(x_0,t_0) e^{i[k(x-x_0)-\omega(t-t_0)]} \right]. \quad (2.43)$$

Changing the order of integration, this expression may be rewritten in the following general form:

$$\Psi(x,t) = \int G(x,t;x_0,t_0) \Psi(x_0,t_0) dx_0, \quad (2.44)$$

where function $G$, usually called kernel in mathematics, in quantum mechanics is called the propagator.$^9$ According to Eq. (43), in our particular case of a free particle the propagator is equal to

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$^9$ Its standard notation by letter $G$ stems from the fact that the propagator is essentially the spatial-temporal Green’s function of Eq. (2.18), defined very similarly to Green’s functions of other ordinary and partial differential equations describing various physics systems – see, e.g., CM Sec. 4.1 and/or EM Sec. 2.7 and 7.3.
The physical sense of the propagator may be understood by considering the following special initial conditions:

\[ \Psi(x_0, t_0) = \delta(x_0 - x'), \quad (2.46) \]

where \( x' \) is a certain point within the domain of particle’s motion. In this particular case, Eq. (44) evidently gives

\[ \Psi(x, t) = G(x, t; x', t_0). \quad (2.47) \]

Hence, the propagator, considered as a function of \( x \) and \( t \) only, is just the solution of the linear differential equation with \( \delta \)-functional initial conditions. Thus while Eq. (41) may be understood as a mathematical expression of the linear superposition principle in the momentum (i.e., reciprocal) space domain, Eq. (44) is an expression of this principle in the direct space domain: the system’s “response” \( \Psi(x, t) \) to an arbitrary initial condition \( \Psi(x_0, t_0) \) is just a sum of its responses to its thin spatial “slices”, with propagator \( G(x, t; x_0, t_0) \) representing the weight of each slice in the final sum.

Calculating integral (45), one should remember that \( \omega \) is not a constant but a function of \( k \), given by the dispersion relation for particular waves. In particular, for the de Broglie waves

\[ G(x, t; x_0, t_0) = \frac{1}{2\pi} \int \exp\left\{ i \left[ k(x - x_0) - \frac{\hbar k^2}{2m} (t - t_0) \right] \right\} dk. \quad (2.48) \]

This is a Gaussian integral again, and may be readily calculated just it was done (twice) above, by completing the exponent to the full square. The result is

\[ G(x, t; x_0, t_0) = \left( \frac{m}{2\pi\hbar(t - t_0)} \right)^{1/2} \exp\left\{ -\frac{m(x - x_0)^2}{2\hbar(t - t_0)} \right\}. \quad (2.49) \]

Please note the following features of this complex function (plotted in Fig. 2):

10 Note that this initial condition is not equivalent to a \( \delta \)-functional initial probability density (2).
(i) It depends only on differences \((x - x_0)\) and \((t - t_0)\). This is natural, because the free-particle propagation problem is uniform (\textit{translation-invariant}) both in space and time.

(ii) The function shape does not depend on its arguments – they just rescale the same function: its snapshot (Fig. 2), if plotted as a function of un-normalized \(x\), just becomes broader and lower with time. It is curious that the spatial broadening scales as \((t - t_0)^{1/2}\) – just as at the classical diffusion, as a result of a deep analogy between quantum mechanics and classical statistics – to be discussed further in Chapter 7.

(iii) In accordance with the uncertainty relation, the ultimately compressed wave packet \((46)\) has an infinite width of momentum distribution, and the quasi-sinusoidal tails of the free-particle propagator, clearly visible in Fig. 2, are the results of the free propagation of the fastest (highest-momentum) components of that distribution, in both directions from the packet center. In the following sections, we will mostly focus on the spatial distribution of stationary, monochromatic wavefunctions (that, for unconfined motion, may be interpreted as wave packets of very large spatial width \(\delta x\)), only rarely coming back to the wave packet discussion. Our excuse is the linear superposition principle, i.e. our conceptual ability to restore the general solution from that of monochromatic waves of all possible energies. However, the reader should not forget that, as the above discussion has illustrated, mathematically this restoration is not always trivial.

### 2.3. Particle motion in simple potential profiles

Now, let us proceed to the cases in which the potential energy \(U(x,t)\) is not identically equal to zero. The easiest case is that of spatially-uniform but time-dependent potential: \(U = U(t) = \text{const.}\). Indeed, the corresponding Schrödinger equation (1.25) with Hamiltonian

\[
\hat{H} = \frac{\hat{p}^2}{2m} + U(t) = -\frac{\hbar^2}{2m} \nabla^2 + U(t),
\]

allows the variable separation similar to that performed in Sec. 1.5, besides that the time-dependent function \(T(t)\) obeys an equation of motion that is slightly more general than Eq. (1.59):

\[
i\hbar \frac{\partial}{\partial t} \hat{T} = [E - U(t)]\hat{T},
\]

whose solution may be expressed as an evident generalization of Eq. (1.61):

\[
T(t) = T(0)e^{-i[\omega t + \varphi(t)]}, \quad \text{with } \omega = \frac{E}{\hbar} \quad \text{and} \quad \frac{d\varphi}{dt} = -\frac{U(t)}{\hbar}.
\]

Looking at the basic relations (1.22) and (1.23) of wave mechanics, it seems that this additional phase factor does not affect the particle probability distribution, or even any observable (including energy it is referred to the instant value of \(U\)), and hence the phase increment \(\varphi\), associated with \(U(t)\), is just a mathematical artifact. This is certainly true for a single particle, however, the situation changes as soon as we recall that the Universe consists of more than one of them.

For example, consider two similar, independent particles, each in the same (say, ground) eigenstate, but with the potential energies (and hence eigenenergies \(E_{1,2}\)) different by a constant \(\Delta U \equiv U_1 - U_2\). Then, the difference \(\varphi \equiv \varphi_1 - \varphi_2\) of their wavefunction phases evolves in time as
If the particles are in different worlds (or at least in different laboratories :-), this evolution is unobservable; however, it should be intuitively clear that a very weak coupling of a certain detector to each particle may allow it to observe phase $\varphi$, while keeping the particle dynamics virtually unperturbed, i.e. Eq. (53) intact.

Perhaps the most dramatic demonstration of this phenomenon is the Josephson effect in superconductors.\(^{11}\) Experimentally, the easiest way to observe the effect is by connecting two bulk superconductor samples with a weak, short electric contact (called either the weak link or the Josephson junction) and bias them with a constant (dc) voltage $V$, typically in a few-microvolt range – see Fig. 3.

Superconductivity may be explained by a specific coupling between its conduction electrons, that leads, at low temperatures, to formation of the so-called Cooper pairs. Such pairs, each consisting of two electrons with opposite spins and momenta, behave as Bose particles, and form coherent Bose-Einstein condensate.\(^{12}\) Most properties of such a condensate may be described by a single wavefunction, evolving in time as that of a free particle with the effective potential energy $U = q\phi = -2e\phi$, where $\phi$ is the electrochemical potential,\(^{13}\) and $q = -2e$ is the total charge of the Cooper pair. As a result, for the situation shown in Fig. 3, Eq. (53) takes the form

$$\frac{d\varphi}{dt} = \frac{2e}{\hbar} V,$$

where $V = \phi_1 - \phi_2$ is the applied voltage. B. Josephson has predicted that, in a particular case when a weak link is a tunnel junction, electric current $I$ of Cooper pairs through it should have a simple form:\(^{14}\)

$$I = I_c \sin \varphi,$$
where $I_c$ is some constant (scaling as the weak link strength). Combining Eqs. (53) and (54), we see that if the applied voltage is constant in time, the current oscillates with the so-called *Josephson frequency*

$$f_J = \frac{\omega_J}{2\pi}, \quad \text{where} \quad \omega_J = \frac{2eV}{\hbar},$$

as high as $\sim 484$ MHz per each microvolt of applied dc voltage. This effect is now well documented, though a direct detection of the Josephson radiation is tricky; it is much easier to observe the *phase locking* (synchronization)$^{15}$ of the radiation by external microwave signal, which results in formation of nearly flat dc current steps at dc voltages

$$V_n = n \frac{\hbar \omega}{2e},$$

where $\omega$ is the external signal frequency and $n$ is an integer.$^{16}$ This effect is now being used in highly accurate standards of dc voltage.$^{17}$

Now, let us move on to a discussion of the opposite case, when a 1D particle modes in various potential profiles $U(x)$ that are constant in time. Conceptually, the simplest of such profiles is a potential step – see Fig. 4.

As I am sure the reader knows, in classical mechanics, if a particle is incident on such a step (in Fig. 4, from the left), its kinetic energy $p^2/2m$ cannot be negative, so that it can only travel through the *classically accessible* region where its (conserved) full energy,

$$E = \frac{p^2}{2m} + U(x),$$

is larger than the local value $U(x)$. Let the initial velocity $v = p/m$ be positive, i.e. directed toward the step. Before it has reached the *classical turning point* $x_c$, defined by equation

$$U(x_c) = E,$$

$^{15}$ See, e.g., CM Sec. 4.4.

$^{16}$ If $\omega$ is not too high, this effect may be adequately described combining Eqs. (54)-(55). Let me leave this task for the reader.

$^{17}$ The most precise proof that the Josephson frequency-to-voltage ratio $f_J/V$ does not depend on superconducting material (to at least 15 decimal places!) has been carried out by the group led by J. Lukens here at Stony Brook – see J.-S. Tsai *et al.*, *Phys. Rev. Lett.* 51, 316 (1983).
kinetic energy $p^2/2m$ never turns to zero, so that the particle continues to move in the initial direction. On the other hand, the particle cannot penetrate that classically forbidden region $x > x_c$, because there its kinetic energy would be negative there. At the point $x = x_c$, particle’s velocity changes sign, i.e. it is reflected back from the classical turning point.

In order to see what the wave mechanics says about this situation, let us start from the simplest, sharp potential step shown with bold black lines in Fig. 5:

$$U(x) = U_0 \theta(x) = \begin{cases} 0, & \text{at } x < 0, \\ U_0, & \text{at } 0 < x. \end{cases} \quad (2.60)$$

For this choice, and any energy within the interval $0 < E < U_0$, the classical turning point is $x_c = 0$.

Let us represent an incident particle with a wave packet so long that the spread $\delta k \sim 1/\delta x$ of its wave number spectrum, and hence the energy uncertainty $\delta E = \hbar \delta \omega = \hbar (d\omega/dk) \delta k$ is negligible in comparison with its average value $E < U_0$, as well as with $(U_0 - E)$. In this case, $E$ may be considered a given constant, and the time dependence of the solution is given by Eq. (1.61), and we can limit ourselves to the solution of the 1D version of the stationary Schrödinger equation (1.63), in this case

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + U(x)\psi = E\psi, \quad (2.61)$$

for the spatial part $\psi(x)$ of the wavefunction.\(^{18}\)

At $x < 0$, i.e. at $U = 0$, the equation is reduced to the Helmholtz equation (1.75), and may be satisfied with two traveling waves, proportional to $\exp\{+ikx\}$ and $\exp\{-ikx\}$ correspondingly, with $k$ satisfying the dispersion equation (1.30):

$$k^2 = \frac{2mE}{\hbar^2}. \quad (2.62)$$

Thus the general solution of Eq. (61) in this region may be presented as

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\(^{18}\) Note that this is not the eigenproblem like the one we have solved in Sec. 1.4 for a quantum well. Indeed, now energy $E$ is considered fixed -- e.g., by the initial conditions that launch a long wave packet upon the potential step, from the left.
The second term in the right-hand part evidently describes an (infinitely long) wave packet traveling to the left, which represents particle’s reflection from the potential step. If $B = -A$, this solution is reduced to Eq. (1.76) for the potential well with infinitely high walls, but as we will see in a minute, for our current case of finite step height $U_0$, the relation between coefficients $B$ and $A$ may be different.

To show this, let us solve Eq. (61) for $x > 0$, where $U = U_0 > E$. In this region the equation may be rewritten as

$$\frac{d^2 \psi_+}{dx^2} = \kappa^2 \psi_+, \quad (2.64)$$

where $\kappa$ is a real constant defined by the relation similar to Eq. (62):

$$\kappa^2 \equiv \frac{2m(U_0 - E)}{\hbar^2} > 0. \quad (2.65)$$

The general solution of Eq. (64) is the sum of $\exp\{+\kappa x\}$ and $\exp\{-\kappa x\}$, with arbitrary coefficients. However, the wavefunction should be finite at $x \to \infty$, so only the latter exponent is acceptable:

$$\psi_+(x) = Ce^{-\kappa x}. \quad (2.66)$$

This penetration of the wavefunction into the classically forbidden region, and hence a finite probability to find the particle there, is one of the most fascinating predictions of quantum mechanics, and has been repeatedly observed in experiment, e.g., via tunneling experiments – see below. From Eq. (66), it is evident that the constant $\kappa$, defined by Eqs. (65), may be interpreted as the reciprocal penetration depth. Even for the lightest particles this depth is usually very small. Indeed, for $E << U_0$ that equation yields

$$\delta \equiv \frac{1}{\kappa} \bigg|_{E=0} = \frac{\hbar}{(2mU_0)^{1/2}}. \quad (2.67)$$

For example, for a conduction electron in a typical metal, that runs, at its surface, into a sharp potential step $U_0$, whose height equals to metal’s workfunction $W \approx 5$ eV (see the discussion of the photoelectric effect in Sec. 1.1), $\delta$ is close to 0.1 nm, i.e. is close to a typical size of an atom. For heavier elementary particles (e.g., protons) the penetration depth is correspondingly lower, and for macroscopic bodies it is hardly measurable.

Returning to our problem, we still should find coefficients $A$, $B$, and $C$ from the boundary conditions at $x = 0$. Since $E$ is a finite constant, and $U(x)$ is a finite function, Eq. (61) says that $d^2 \psi/dx^2$ should be finite as well. This means that the first derivative should be continuous:

$$\lim_{\varepsilon \to 0} \left( \frac{d \psi}{dx} \bigg|_{x=+\varepsilon} - \frac{d \psi}{dx} \bigg|_{x=-\varepsilon} \right) = \lim_{\varepsilon \to 0} \int_{-\varepsilon}^{+\varepsilon} \frac{d^2 \psi}{d^2x} \, dx = \lim_{\varepsilon \to 0} \int_{-\varepsilon}^{+\varepsilon} \left[ U(x) - E \right] \psi \, dx = 0. \quad (2.68)$$

Repeating such calculation for function $\psi(x)$ itself, we see that it also should be continuous at all points, including $x = 0$, so that
\[ \psi_-(0) = \psi_+(0), \quad \frac{d\psi_-}{dx}(0) = \frac{d\psi_+}{dx}(0). \quad (2.69) \]

Plugging solutions (63) and (66) into these two boundary conditions, we get a system of two linear equations

\[ A + B = C, \quad ikA - ikB = -\kappa C, \quad (2.70) \]

whose (elementary) solution enables us to express \( B \) and \( C \) via \( A \):

\[ B = A \frac{k - i\kappa}{k + i\kappa}, \quad C = A \frac{2k}{k + i\kappa}. \quad (2.71) \]

We immediately see that since the numerator and denominator in the first of these formulas have equal moduli, so that \(|B| = |A|\). This means that, as we could expect, a particle with energy \( E < U_0 \) is totally reflected from the step. As a result, at \( x < 0 \) our solution (63) may be presented by a standing wave

\[ \psi_- = 2iAe^{i\theta} \sin(kx - \theta), \quad \text{with} \quad \theta = \tan^{-1} \frac{k}{\kappa}. \quad (2.72) \]

Notice that the shift \( \Delta x \equiv \theta k = (\tan^{-1} k/\kappa)/k \) of the standing wave to the right, due to the partial penetration of the wavefunction under the potential step, is commensurate with, but generally not equal to \( \delta \equiv 1/k \). Figure 5 shows the full behavior of the wavefunction, for a particular case \( E = U_0/5 \), at which \( k/\kappa = \left[ E/(U_0-E) \right]^{1/2} = 1/2 \).

According to Eq. (65), as the particle’s energy \( E \) is increased to approach \( U_0 \), the penetration depth \( 1/\kappa \) diverges. This raises an important issue: what happens at \( E > U_0 \), i.e. if there is no classically forbidden region in the problem? Again, in classical mechanics the incident particle would continue to move to the right, though with a reduced velocity, corresponding to the new kinetic energy \( E - U_0 \), so there would be no reflection. In quantum mechanics, however, the situation is different. In order to analyze it, it is not necessary to re-solve the whole problem; it is sufficient to note that all our calculations, and hence Eqs. (71) are still valid if we take\(^{19}\)

\[ \kappa = -ik', \quad \text{with} \quad k'^2 \equiv \frac{2m(E-U_0)}{\hbar^2} > 0. \quad (2.73) \]

With this replacement, Eq. (71) becomes\(^{20}\)

\[ B = A \frac{k - k'}{k + k'}, \quad C = A \frac{2k}{k + k'}. \quad (2.74) \]

The most important result of this change is that now the reflection is not complete: \(|B| < |A|\). In order to evaluate this effect qualitatively, it is more fair to use not the \( B/A \) or \( C/A \) ratios, but rather that

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\(^{19}\) Our earlier discarding of the particular solution \( \exp\{\kappa x\} \), now becoming \( \exp\{-ik'x\} \), is still valid, but now on a different grounds: this term would describe a wave packet incident on the potential step from the right, and this is not the problem under our consideration.

\(^{20}\) These formulas are completely similar to those for the partial reflection of classical waves from a sharp interface between two uniform media, at normal incidence (see, e.g., CM Sec. 5.4 and EM Sec. 7.4), with the effective impedance \( Z \) of de Broglie waves proportional to their wave number \( k \).
of the probability currents (5) corresponding to traveling waves with amplitudes $C$ and $A$, in the corresponding regions (respectively, $x > 0$ and $x < 0$):

$$T = \frac{I_C}{I_A} = \frac{k |C|^2}{k |A|^2} = \frac{4k'k}{(k + k')^2} = \frac{4[E(E - U_0)]^{1/2}}{[E^{1/2} + (E - U_0)^{1/2}]^2}. \quad (2.75)$$

($T$ so defined is called the transparency of the inhomogeneity, in our current case of the potential step.) The result given by Eq. (75) is plotted in Fig. 6a. Notice its most important features:

(i) At $U_0 = 0$, the transparency is full, $T = 1$ – naturally, for having no step at all.

(ii) At $U_0 \to E$, the transparency tends to zero - giving a proper connection with the case $E < U_0$.

(iii) We can use result (75) even for $U_0 < 0$, i.e. for the step-down (or “cliff”) profile – see Fig. 6b. Very counter-intuitively, the particle is (partly) reflected even from such a cliff, and the transmission diminishes (rather slowly) at $U_0 \to -\infty$.

The most important conceptual conclusion of our analysis is that the quantum particle is partly reflected from a potential step with $U_0 < E$, in the sense that there is a nonvanishing probability $T < 1$ to find it passed over the step, while there is also probability $(1 - T)$ to have it reflected.

The same property is exhibited, for any relation between $E$ and $U_0$, by another simple potential profile $U(x)$, the famous tunnel barrier. Figure 7 shows its simple, “rectangular” version:

$$U(x) = \begin{cases} 
0, & \text{for } x < -d/2, \\
U_0, & \text{for } -d/2 < x < +d/2, \\
0, & \text{for } +d/2 < x.
\end{cases} \quad (2.76)$$

Fig. 2.7. Rectangular tunnel barrier.
In order to analyze this problem, it is sufficient to look for the solution to the Schrödinger equation in the form (63) at \( x \leq -d/2 \). At \( x > +d/2 \), i.e., behind the barrier, we may use the arguments presented above (no wave packet source on the right!) to keep just one traveling wave,

\[
\psi_+(x) = Fe^{ikx}.
\]  
(2.77)

However, under the barrier, i.e. at \(-d/2 \leq x \leq +d/2\), we should generally keep both exponential terms,

\[
\psi_b(x) = Ce^{-\kappa x} + De^{+\kappa x},
\]  
(2.78)

because our previous argument, used in the potential step problem’s solution, is no longer valid. (Here \( k \) and \( \kappa \) are still defined, respectively, by Eqs. (62) and (65).) In order to find the relation between coefficients \( A, B, C, D, \) and \( F \), we need to plug in the solutions into the boundary conditions similar to Eqs. (69), but now at two boundary points, \( x = \pm d/2 \).

Solving the resulting system of 4 linear equations for five amplitudes \( (A, B, C, D, \) and \( F \)), we can readily calculate four ratios \( B/A, C/A, \) etc., in particular,

\[
\frac{F}{A} = \frac{\exp\left[-ikd\right]}{\cosh kd + \frac{i}{2} \left( \frac{\kappa}{k} - \frac{k}{\kappa} \right) \sinh kd},
\]  
(2.79a)

and hence barrier’s transparency

\[
T = \left| \frac{F}{A} \right|^2 = \left[ \cosh^2 \kappa d + \left( \frac{\kappa^2 - k^2}{2\kappa k} \right)^2 \sinh^2 \kappa d \right]^{-1}.
\]  
(2.79b)

Figure 8a shows the transparency as a function of particle energy \( E \), for several characteristic values of the barrier thickness \( d \), or rather of the ratio \( d/\delta \), where \( \delta \) is defined by Eq. (67).
The plots show that for a thin barrier \((d < \delta)\) the transparency grows gradually with particle’s energy. This growth is natural, because the penetration constant \(\kappa\) decreases with the growth of \(E\), i.e., the wavefunction penetrates more and more into the barrier, so that more and more of it is “picked up” at the second interface \((x = +d/2)\) and transferred into the wave \(F \exp\{ikx\}\) propagating behind the barrier. As Eq. (79b) shows, for thick barriers \((d >> \delta)\), this dependence is dominated by an exponent,

\[
T \approx \left( \frac{4k\kappa}{k^2 + \kappa^2} \right)^2 e^{-2\kappa d}, \tag{2.80}
\]

that may be clearly seen as a straight segments in semi-log plots (Fig. 8b) of \(T\) as a function of the combination \((1 – E/U_0)^{1/2}\) which is proportional to \(\kappa\) - see Eq. (65).

Equation (80) also clearly shows the exponential dependence of the barrier transparency of its thickness at \(d >> \delta\). This dependence is the most important factor for various applications of the quantum-mechanical tunneling – from the field emission\(^{21}\) of electrons to scanning tunneling microscopy.\(^{22}\) Also noted should be substantial negative implications of the effect for modern electronic engineering, most importantly imposing a limit for scaling down of field effect transistors in semiconductor integrated circuits (and hence the circuit density increase according to the well-known Moore’s law), due to increase of tunneling both through the gate oxide and along transistor’s channel.\(^{23}\)

Another interesting effect visible in Fig. 8a (for case \(d = 0.3\delta\)) are the oscillations of \(T\) at \(E > U_0\). This is our first glimpse at one more interesting quantum effect: resonant tunneling. I will discuss this effect in detail in Sec. 5 below.

### 2.4. The WKB approximation

Before moving on to exploring more complex potentials, let us see whether the results discussed in the previous section hold on in the opposite limit of so-called soft, gradual potential profiles, like that sketched in Fig. 4. (The quantitative conditions of the “softness” will be derived below). The most efficient analytical tool in this limit is the WKB (or “quasiclassical”) approximation developed by H. Jeffrey, G. Wentzel, A. Kramers, and L. Brillouin in 1926-27.

In order to derive its 1D version, let us rewrite the Schrödinger equation (61) as

\[
\frac{d^2\psi}{dx^2} + k^2(x)\psi = 0 \tag{2.81}
\]

where the local value of wave number \(k(x)\) is defined similarly to Eq. (73),

\[
k^2(x) \equiv \frac{2m[E - U(x)]}{\hbar^2}, \tag{2.82}
\]

but now it may be a function of \(x\). We already know that for \(k(x) = \text{const}\), the fundamental solutions of this equation have form \(A \exp\{+ikx\}\) and \(B \exp\{-ikx\}\). Any of them may be presented in a simple form

\[ \psi(x) = e^{i \Phi(x)}, \quad (2.83) \]

where \( \Phi(x) \) is a complex function, in this simplest case equal to either \((kx - i \ln A)\) or \((-kx - i \ln B)\). This is why we may try use Eq. (83) to look for solution of Eq. (81) even in the general case, \( k(x) \neq \text{const.} \)

Differentiating Eq. (83) twice, we get

\[
\frac{d\psi}{dx} = i \frac{d\Phi}{dx} e^{i \Phi}, \quad \frac{d^2 \psi}{dx^2} = \left[ i \frac{d^2 \Phi}{dx^2} - \left( \frac{d\Phi}{dx} \right)^2 \right] e^{i \Phi}. \quad (2.84)
\]

Plugging the last expression into Eq. (81) and requiring the factor before \( \exp\{i \Phi(x)\} \) to vanish, we get

\[
\frac{i}{k^2} \frac{d^2 \Phi}{dx^2} + k^2(x) = 0. \quad (2.85)
\]

This is still an exact, general result. At the first sight, it looks worse than the initial equation (81), because Eq. (85) is nonlinear. However, it is more ready for simplification in the limit when the potential profile is very smooth, \( dU/dx \to 0 \). Indeed, we know that for a uniform potential, \( \Phi'' = 0 \). Hence, in the “0th” approximation, \( \Phi(x) \to \Phi_0(x) \), we may try to keep that result, so that Eq. (85) yields

\[
\left( \frac{d\Phi_0}{dx} \right)^2 = k^2(x). \quad (2.86a)
\]

Just as in the uniform case, this equation has two roots,

\[
\frac{d\Phi_0}{dx} = \pm k(x), \quad (2.86b)
\]

so that its general solution is

\[
\psi_0(x) = A \exp\left\{ + i \int k(x') dx' \right\} + B \exp\left\{ - i \int k(x') dx' \right\}, \quad (2.87)
\]

where \( x' \) is the lower limits of integration affect only constants \( A \) and \( B \). The physical sense of this result is simple: it is a sum of forward- and back-propagating waves, with the coordinate-dependent local wave number \( k(x) \) that self-adjusts to the potential profile.

Let me emphasize the non-trivial nature of this approximation.\(^{24}\) First, any attempt to address the problem with a standard perturbation approach (say, \( \psi = \psi_0 + \psi_1 + \ldots \), with \( \psi_n \) proportional to \( n^{\text{th}} \) power of some small parameter,\(^{25}\) in this case scaling \( d^2 U/d^2 x \) would fail for most potentials, because even a slight but persisting deviation of \( U(x) \) from a constant leads to a gradual accumulation of phase \( \Phi_0 \), impossible to describe by any small perturbation of \( \psi \). Second, the dropping of term \( d^2 \Phi/dx^2 \) in Eq. (85) is not too easy to justify. Indeed, since we are committed to the “soft potential limit” \( dU/dx \to 0 \), we should be ready to assume the characteristic length \( a \) of spatial variation of \( \Phi \) to be large, and neglect

\(^{24}\) Philosophically, this space-domain method is very close to the time-domain rotating wave approximation (RWA) used, for example, in the classical and quantum theory of oscillations – see, e.g., CM Secs. 4.2-4.5, and Secs. 6.5, 7.6, 7.7, 9.2, and 9.4 of this course.

\(^{25}\) Such perturbation theories will be discussed in Chapter 6.
the terms that are the smallest ones in the limit \( a \to \infty \). However, both first terms in Eq. (85) are apparently of the same order in \( a \), namely \( O(a^{-2}) \); why have we neglected just one of them?

The price we have paid for such a “sloppy” treatment is high: Eq. (87) does not satisfy the fundamental property of the Schrödinger equation, the probability current conservation. Indeed, since Eq. (81) describes a fixed-energy (stationary) spatial part of the general Schrödinger equation, its probability density \( w = \Psi \Psi^* = \psi \psi^* \), and should not depend on time. Hence, according to Eq. (6), we should have \( I(x) = \text{const.} \). However, this is not true for each component of Eq. (87); for example for the forward-propagating component of its right-hand part, Eq. (5) yields

\[
I_0(x) = \frac{\hbar}{m} |A|^2 k(x),
\]

evidently not a constant if \( k(x) \neq \text{const.} \).

The brilliance of the WKB theory is that the problem may be fixed without revising the 0\(^{th}\) approximation. Indeed, let us explore the next, 1\(^{st}\) approximation instead:

\[
\Phi(x) \to \Phi_{\text{WKB}}(x) \equiv \Phi_0(x) + \Phi_1(x),
\]

where \( \Phi_0 \) still obeys Eq. (85), while \( \Phi_1 \) describes a small correction to the 0\(^{th}\) approximation, in the following sense:\(^{26}\)

\[
\left| \frac{d\Phi_1}{dx} \right| \ll \left| \frac{d\Phi_0}{dx} \right| = k(x).
\]

Plugging Eq. (89) into Eq. (85), with the account of the definition (86), we get

\[
i \left( \frac{d^2\Phi_0}{dx^2} + \frac{d^2\Phi_0}{dx^2} \right) - \frac{d}{dx} \left( 2 \frac{d\Phi_0}{dx} + \frac{d\Phi_1}{dx} \right) = 0.
\]

Using condition (90), we may neglect \( d^2\Phi_1/dx^2 \) in comparison with \( d^2\Phi_0/dx^2 \) in the first parenthesis, and \( d\Phi_1/dx \) in comparison with \( 2d\Phi_0/dx \) in the second parenthesis. As a result, we get the following approximate result:

\[
\frac{d\Phi_1}{dx} = \frac{i}{2} \frac{d^2\Phi_0}{dx^2} = \frac{i}{2} \frac{d}{dx} \left( \ln \frac{d\Phi_0}{dx} \right) = \frac{i}{2} \frac{d}{dx} \left[ \ln k(x) \right] = \frac{i}{2} \frac{d}{dx} \left[ \ln k^{1/2}(x) \right],
\]

\[
\left. i\Phi \right|_{\text{WKB}} = i\Phi_0 + i\Phi_1 = \pm i \int x k(x')dx' + \ln \frac{1}{k^{1/2}(x)},
\]

\[
\psi_{\text{WKB}}(x) = \frac{a}{k^{1/2}(x)} \exp \left\{ \frac{i}{2} \int \frac{1}{k(x')} dx' \right\} + \frac{b}{k^{1/2}(x)} \exp \left\{ -i \frac{1}{2} \int \frac{1}{k(x')} dx' \right\}, \quad \text{for } k^2(x) > 0.
\]

(Again, the lower integration limit is arbitrary, but its choice may be incorporated into complex constants \( a \) and \( b \).) This modification of the 0\(^{th}\) approximation (87) overcomes the problem of current continuity; for example, for the forward-propagating wave, Eq. (5) gives

---

\(^{26}\) For certainty, I will use the discretion given by Eq. (82) to define \( k(x) \) as the positive root of its right-hand part.
\[ I_{\text{WKB}}(x) = \frac{\hbar}{m} |a|^2 = \text{const.} \] (2.95)

Physically, factor \( k^{1/2} \) in the denominator of the WKB wavefunction’s pre-exponent is easy to understand. The smaller the local group velocity (34) of the wave packet, \( v_{\text{gr}}(x) = \hbar k(x)/m \), the “easier” (more probable) it should be to find the particle within a certain interval \( dx \). This is exactly the result that WKB gives: \( dW/dx = w(x) = \psi\psi^* \propto 1/k(x) \propto 1/v_{\text{gr}} \).

Another value of the 1st approximation is a clarification of WKB theory’s validity condition: it is given by Eq. (90). Plugging into this relation the first form of Eq. (92), and estimating \( |\Phi_0^*| \) as \( |\Phi_0|/a \), where \( a \) is the spatial scale of a substantial change of \( |\Phi_0| = k(x) \), we can rewrite the condition as

\[
ka \gg 1. \quad (2.96)
\]

In plain English, this means that the region where \( U(x) \), and hence \( k(x) \), change substantially should contain many de Broglie wavelengths \( \lambda = 2\pi/k \).

So far I have implied that \( k^2(x) \propto E - U(x) \) is positive, i.e. particle moves in the classically accessible region. Now let us extend the WKB approximation to the situation where the difference \( E - U(x) \) may change sign, for example to the reflection problem sketched in Fig. 4. Just as we did for the sharp potential step, we first need to find the appropriate solution for the classically forbidden region, in this case \( x > x_c \). For that, there is no need to redo our calculations, because they are still valid if we, just as in the sharp step problem, take \( k(x) = i\kappa(x) \), where

\[
\kappa^2(x) = \frac{2m[U(x) - E]}{\hbar^2} > 0, \quad \text{for} \ x > x_c, \quad (2.97)
\]

and keep just one of two possible solutions (with \( \kappa > 0 \)), in analogy with Eq. (66). The result is

\[
\psi_{\text{WKB}}(x) = \left( \frac{c}{\kappa^{1/2}(x)} \right) \exp \left\{ -\frac{\kappa(x')dx'}{2} \right\}, \quad \text{for} \ k^2 < 0, \ i.e. \ \kappa^2 > 0, \quad (2.98)
\]

with the lower limit at some point with \( \kappa^2 > 0 \) as well. This is a really wonderful formula! It describes the quantum-mechanical penetration of the particle into the classically forbidden region, and provides a natural generalization of Eq. (66) - leaving intact, of course, our estimates of the depth \( \delta \sim 1/\kappa \) of such penetration.

Now we have to do what we have done for the sharp-step problem in Sec. 2: use the boundary conditions in the interface point \( x = x_c \) to relate constants \( a, b, \) and \( c \). However, now this operation is a tad more complex, because both WKB functions (94) and (98) diverge, albeit weakly, at the classical turning point, were both \( k(x) \) and \( \kappa(x) \) tend to zero. This connection problem may be however, solved in the following way. \(^{27}\) Let us use the commitment of potential “softness”, assuming that it allows us to keep just two leading terms in the Taylor expansion of function \( U(x) \) at point \( x_c \):

\[
U(x) \approx U(x_c) + \left. \frac{dU}{dx} \right|_{x=x_c} (x-x_c) = E + \left. \frac{dU}{dx} \right|_{x=x_c} (x-x_c). \quad (2.99)
\]

\(^{27}\) An alternative way to solve the connection problem, without involving the Airy functions but using an analytical extension of WKB formulas to the plane of complex argument, may be found, e.g., in Sec. 47 of textbook by L. Landau and E. Lifshitz, Quantum Mechanics, Non-Relativistic Theory, 3rd ed. Pergamon, 1977.
Using this truncated expansion, and introducing a dimensionless variable for coordinate’s deviation from the classical turning point,
\[
\zeta \equiv \frac{x - x_c}{x_0}, \quad x_0 = \left(\frac{\hbar^2}{2m(dU/dx)}\right)^{1/3},
\]
we reduce the Schrödinger equation (61) to the simple Airy equation
\[
\frac{d^2\psi}{d\zeta^2} - \zeta \psi = 0.
\]
(2.100) Airy equation

As for all linear, ordinary differential equations of the second order, the general solution of Eq. (101) may be presented as a linear combination of two fundamental solutions, in this case called Airy functions \(\text{Ai}(\zeta)\) and \(\text{Bi}(\zeta)\), shown in Fig. 9a.

![Fig. 2.9. (a) Airy functions Ai and Bi, and (b) the WKB approximation for function Ai(\(\zeta\)).](image)

The latter function diverges at \(\zeta \to \infty\), and thus is not suitable for our current problem (Fig. 4), while the former function has the following asymptotic behaviors at \(|\zeta| \gg 1\): 28
\[
\text{Ai}(\zeta) \to \frac{1}{\pi^{1/2} |\zeta|^{1/4}} \times \begin{cases} 
\frac{1}{2} \exp\left(-\frac{2}{3} \zeta^{3/2}\right), & \text{for } \zeta \to +\infty, \\
\sin\left(\frac{2}{3} (-\zeta)^{3/2} + \frac{\pi}{4}\right), & \text{for } \zeta \to -\infty.
\end{cases}
\]
(2.102)

Now let us apply the WKB approximation to the Airy equation (101). Taking the classical turning point \((\zeta = 0)\) for the lower limit, for \(\zeta > 0\) we get (in dimensionless units)

---

28 The following (exact!) integral formulas,
\[
\text{Ai}(\zeta) = \frac{1}{\pi} \int_0^\infty \cos\left(\frac{x^3}{3} + \zeta x\right) dx, \quad \text{Bi}(\zeta) = \frac{1}{\pi} \int_0^\infty \left[\exp\left(-\frac{x^3}{3} + \zeta x\right) + \sin\left(\frac{x^3}{3} + \zeta x\right)\right] dx,
\]
are often convenient for practical calculation of Airy functions at intermediate values of the argument, \(|\zeta| \sim 1\).
\[
\kappa^2 (\zeta') = \zeta, \quad \kappa (\zeta') = \zeta^{1/2}, \quad \int_0^\zeta \kappa (\zeta') d\zeta' = \frac{2}{3} \zeta^{3/2}, \tag{2.103}
\]
i.e. exactly the exponent in the first line of Eq. (102). Making a similar calculation for \( \zeta < 0 \), with the natural assumption \(|b| = |a|\) (full reflection from the potential step), we arrive at the following result:

\[
\text{Ai}_{\text{WKB}} (\zeta) = \frac{1}{|\zeta|^{1/4}} \begin{cases} 
    c \exp \left( -\frac{2}{3} \zeta^{3/2} \right), & \text{for } \zeta > 0, \\
    a \sin \left( \frac{2}{3} (-\zeta)^{3/2} + \varphi \right), & \text{for } \zeta < 0.
\end{cases} \tag{2.104}
\]

This approximation differs from the exact solution at small values of \( \zeta \), i.e. close to the classical turning point – see Fig. 9b. However, at \(|\zeta| >> 1\), Eqs. (104) describe the Airy function exactly if

\[
\varphi = \frac{\pi}{4} \quad \text{and} \quad c = \frac{a}{2}. \tag{2.105}
\]

Hence we can use these connection formulas to express the relations between coefficients \( a, b, \) and \( c \) of the general WKB solutions (94) and (98). In particular, the first of them yields \( b = -a \exp \{i\pi/2\} \), so that Eq. (94) becomes

\[
\psi_{\text{WKB}} (x < x_c) = \frac{a'}{k^{1/2} (x)} \left[ \exp \left( \frac{x}{x_c} k(x')dx' \right) - \exp \left( -\frac{x}{x_c} k(x')dx' + i\frac{\varphi}{2} \right) \right]. \tag{2.106}
\]

This result may be also described by a simple mnemonic rule: reflecting from a “soft” potential step, the wavefunction acquires an additional phase shift \( \Delta \varphi = \pi/2 \), if compared with the reflection from a “hard” (vertical) potential wall located at \( x = x_c \), for which, according to Eq. (1.76), we would have \( b = -a \).

Let us quantify the condition of validity of the connection formulas (105) - in other words, the criterion of the step “softness”. For that, within the region where the WKB approximation differs from the exact Airy equation (\(|\zeta| \sim 1\), i.e. \(|x - x_c| \sim x_0\)), the deviation from the linear approximation (99) of the potential profile should be relatively small. This deviation may be estimated using the next term of the Taylor expansion, \( d^2U/d^2x \mid_{x=x_c} (x - x_c)^2/2 \). As a result, the softness condition may be expressed as \( \left| \frac{d^2U}{dx^2} \right|_{x=x_c} x_0 \ll \left| \frac{dU}{dx} \right|_{x=x_c} \). With the account of Eq. (100) for \( x_0 \), the condition becomes

\[
\left| \frac{d^2U}{dx^2} \right|_{x=x_c} \ll \frac{2m}{\hbar^2} \left( \frac{dU}{dx} \right)_{x=x_c}^4, \tag{2.107}
\]

As an example of a very useful application of the WKB approximation, let us use it to calculate the energy spectrum of 1D particle in a soft 1D quantum well (Fig. 10). As was discussed above, we may always consider the standing wave describing an eigenstate \( \psi_n \) (corresponding to eigenenergy \( E_n \)) as a traveling wave going back and forth between the walls, being sequentially reflected by each of them. Let us apply the WKB approximation to such a traveling wave. First, according to Eq. (94), propagating from the left classical turning point \( x_L \) to the right point \( x_R \), it acquires phase change

\[
\Delta \varphi \rightarrow = \int_{x_L}^{x_R} k(x) dx. \tag{2.108}
\]
At the reflection from the soft wall at \( x_R \), according to the connection formula (106), the wave acquires an additional shift \( \pi/2 \). Now, traveling back from \( x_R \) to \( x_L \) the wave gets a shift similar to one given by Eq. (108): \( \Delta \varphi_{e-} = \Delta \varphi_{\rightarrow} \). Finally, at the reflection from \( x_L \) it gets one more \( \pi/2 \). Summing up all these contributions, we may write the self-consistency condition (that the wavefunction “catches its own tail with its teeth”), in the form

\[
\Delta \varphi_{\text{total}} \equiv \Delta \varphi_{\rightarrow} + \frac{\pi}{2} + \Delta \varphi_{e-} + \frac{\pi}{2} = 2 \int_{x_L}^{x_R} k(x) dx + \pi = 2n\pi, \quad \text{with } n = 1, 2, \ldots \tag{2.109}
\]

Rewriting this result in terms of particle’s momentum \( p(x) = \hbar k(x) \), we arrive at the famous 1D Bohr-Sommerfeld quantization rule

\[
\oint_C p(x) dx = 2\pi\hbar \left( n - \frac{1}{2} \right), \tag{2.110}
\]

where the closed path \( C \) means the full period of classical motion.\(^{29}\)

Let us see what does this rule give for the very important particular case of a quadratic potential profile of a harmonic oscillator of frequency \( \omega_0 \). In this case,

\[
U(x) = \frac{m}{2} \omega_0^2 x^2, \tag{2.111}
\]

and the classical turning points are the roots of a simple equation

\[
\frac{m}{2} \omega_0^2 x_c^2 = E_n, \tag{2.112}
\]

so that \( x_R = x_n = (2E_n/m)^{1/2}/\omega_0 > 0, x_L = -x_n < 0 \). Due to potential’s symmetry, the integration required by Eq. (110) is also simple:

\[
\int_{x_L}^{x_R} p(x) dx = \int_{x_L}^{x_R} \left[ 2m[E_n - U(x)] \right]^{1/2} dx = (2mE_n)^{1/2} \int_{-x_n}^{+x_n} \left( 1 - \frac{x^2}{x_n^2} \right)^{1/2} dx = (2mE_n)^{1/2} x_n \frac{\pi}{2} = \frac{2E_n \pi}{\omega_0^2}, \tag{2.113}
\]

\(^{29}\)Note that at motion in more than one dimension, a closed classical trajectory may have no turning points. In this case, the constant \( \frac{1}{2} \) in the parentheses of Eq. (109), arising from the turns, should be dropped. The simplest example is the circular motion of the electron about the proton in Bohr’s picture of the hydrogen atom, for which the modified quantization (109) condition takes form (1.10) postulated by N. Bohr. (A similar relation for the radial motion is sometimes called the Sommerfeld-Wilson quantization rule.)
so that Eq. (110) is satisfied if

$$E_n = \hbar \omega_0 \left( n' + \frac{1}{2} \right), \quad \text{with } n' \equiv n - 1 = 0, 1, 2, ....$$

(2.114)

In order to estimate the validity of this result, we have to check condition (96) at all points of the classically allowed region, and Eq. (107) at the turning points. A straightforward calculation shows that both conditions are valid for $n \gg 1$. However, we will see below that Eq. (114) is actually exactly correct for all energy levels — thanks to special properties of potential profile (111).

Now, let us look at the second of connection formulas (105), $c = a/2$. Again, it differs from the result (71) for a sharp potential step, that may be rewritten as

$$C = A \frac{2k}{k + i \kappa} = A \frac{2}{1 + (\kappa/k)^2}^{1/2} \exp\{-i2\theta\},$$

by both the modulus and phase factor. (In the WKB approximation, the latter factor always equals $\pi/4$.) Hence, again, the WKB approximation’s prediction is not exact for sharp potentials; nevertheless, it is broadly used for practical calculations. One of the most important of them is the transparency of an arbitrary but smooth potential barrier (Fig. 11).

Here, just as in the case of a rectangular barrier, we need to take unto consideration five partial “waves” (or rather fundamental solutions of the Schrödinger equation): 30

$$\Psi_{\text{WKB}} = \begin{cases} \frac{a}{k^{1/2}(x)} \exp\left\{i \int k(x')dx'\right\} + \frac{b}{k^{1/2}(x)} \exp\left\{-i \int k(x')dx'\right\}, & \text{for } x < x_c, \\ \frac{c}{k^{1/2}(x)} \exp\left\{-i \int k(x')dx'\right\} + \frac{d}{k^{1/2}(x)} \exp\left\{i \int k(x')dx'\right\}, & \text{for } x_c < x < x_c', \\ \frac{f}{k^{1/2}(x)} \exp\left\{i \int k(x')dx'\right\}, & \text{for } x_c' < x, \end{cases}$$

(2.116)

where lower limits of integrals are arbitrary (each within the corresponding range of $x$). Since on the right of the left classical point we have two exponents rather than one, and on the right of the second

30 Sorry, but the same letter, $d$, is used here for the barrier thickness (defined in this case as the classically forbidden region length, $x_c' - x_c$), and the constant in one of the wave amplitudes — see Eq. (116). Let me hope that the difference between these uses is absolutely evident from the context.
point, one traveling waves rather than two, the connection formulas (105) have to be generalized, using asymptotic formulas not only for $\text{Ai}(\zeta)$, but also for the second Airy function, $\text{Bi}(\zeta)$. The analysis, absolutely similar to that carried out above (though naturally a bit more bulky),\(^{31}\) gives a remarkably simple result:

$$
T_{\text{WKB}} \equiv \left| \frac{f}{a} \right|^2 = \exp \left\{ - \int_{x_c}^{x_c'} \kappa(x) \, dx \right\} = \exp \left\{ - \frac{2}{\hbar} \int_{x_c}^{x_c'} \left( 2m[U(x) - E] \right)^{1/2} \, dx \right\},
$$

(2.117)

with no pre-exponential factor. This formula is broadly used in applied quantum mechanics, despite the approximate character of its pre-exponential coefficient for insufficiently soft barriers that do not satisfy Eq. (107). For example, Eq. (80) shows that for a thick rectangular barrier with $k = \kappa$, i.e. $U_0 = 2E$, the WKB approximation (117) underestimates $T$ by a factor of 4. However, on the logarithmic scale of Fig. 8b, such factor, about half an order of magnitude, still looks as a small correction.

Notice that when $E$ approaches the barrier top $U_{\text{max}}$ (Fig. 11), points $x_c$ and $x_c'$ merge, so that, according to Eq. (117), $T_{\text{WKB}} \to 1$, i.e. the particle reflection vanishes at $E = U_{\text{max}}$. However, this conclusion is incorrect even for smooth barriers where one could naively expect the WKB approximation to work perfectly. Indeed, near point $x = x_m$ where the potential reaches maximum (i.e. $U(x_m) = U_{\text{max}}$), we may always approximate a smooth function $U(x)$ by an inverted parabola,

$$
U(x) \approx U_{\text{max}} - \frac{m \omega_0^2 (x - x_m)^2}{2}.
$$

(2.118)

Calculating the derivatives $dU/dx$ and $d^2U/dx^2$ of this function and plugging them into condition (107), we see that the WKB approximation is only valid if $|U_{\text{max}} - E| > > \hbar \omega_0$. An exact analysis\(^{32}\) of tunneling through barrier (118) gives the following \textit{Kemble formula}:

$$
T = \frac{1}{1 + \exp \left\{ - 2\pi (E - U_{\text{max}}) / \hbar \omega_0 \right\}},
$$

(2.119)

valid for any sign of difference $(E - U_{\text{max}})$. This formula describes a gradual approach of $T$ to 1, i.e. a \textit{gradual} reduction of reflection at particle energy’s increase, with $T = \frac{1}{2}$ (rather than 1) at $E = U_{\text{max}}$.

Now the last remark of this section: our discussions of the propagator and the WKB approximation open a straight way toward an alternative formulation of quantum mechanics, based on the \textit{Feynman path integral}, but I will postpone its discussion until a more compact (“bra-ket”) notation has been introduced in Chapter 4.

### 2.5. Transfer matrix, resonant tunneling, and metastable states

Let us now explore motion in more complex potential profiles. The piecewise-constant and smooth-potential models of $U(x)$ are not too convenient here, because they both require “stitching” local

\(^{31}\) Note, however, that in the most important case $T_{\text{WKB}} << 1$, Eq. (117) may be simply derived from Eqs. (105) – an exercise left for the reader.

\(^{32}\) It was carried out by E. Kemble in 1935. Notice that mathematically the Kemble formula is similar to the Fermi distribution in statistical physics, with effective temperature $T_{ef} = \hbar \omega_0 / 2 \pi \hbar$. This similarity has some interesting implications for the statistics of Fermi gas tunneling.
solutions in each classical turning point, which may lead to very cumbersome calculations. However, we may get a very good insight of the physics phenomena in such profiles, using their approximation by a set of Dirac’s delta-functions. For that, let us have a look at what our old result (79) gives in the limit of a very thin and high rectangular barrier, \( d \ll \delta, E \ll U_0 \) (giving \( k \ll \kappa \ll 1/d \)):

\[
T \equiv \left| \frac{F}{A} \right|^2 \to \frac{1}{|1 + i\alpha|^2} = \frac{1}{1 + \alpha^2},
\]  

(2.120)

where parameter \( \alpha \) is defined as

\[
\alpha \equiv \frac{1}{2} \left( \frac{\kappa^2 - k^2}{\kappa k} \right) \kappa d \approx \frac{1}{2} \frac{k^2 d}{k} \approx \frac{m}{\hbar^2 k} U_0 d.
\]  

(2.121)

The last product, \( U_0 d \), is just the “area”

\[
\omega \equiv \int_{U(x) > E} U(x) dx
\]  

(2.122)

of the barrier. This fact implies that the very simple result (120) for the transparency may be correct for a barrier of any shape, provided that it is sufficiently thin and high.

Indeed, let us consider the tunneling problem for a very thin barrier with \( \kappa d, kd \ll 1 \) (Fig. 12), approximating it by Dirac’s \( \delta \)-function:

\[
U(x) = \omega \delta(x).
\]  

(2.123)

We already know the solutions in all points but \( x = 0 \) – see Eqs. (63) and (77) – so we only need to analyze boundary conditions in that point to find coefficients \( A, B, \) and \( F \)- or rather the ratios \( B/A \) and \( F/A \). However, due to the special character of the \( \delta \)-function, we should be careful here. Indeed, instead of Eq. (68) we now get

\[
\frac{d\psi_+}{dx}(0) - \frac{d\psi_-}{dx}(0) = \lim_{\varepsilon \to 0} \frac{d^2\psi}{dx^2} = \lim_{\varepsilon \to 0} \frac{2m}{\hbar^2} \int_{-\varepsilon}^{\varepsilon} \frac{U(x) - E}{x} \psi \, dx = \frac{2m}{\hbar^2} \omega \psi(0).
\]  

(2.124)

On the other hand, the wavefunction itself is still continuous:

\[
\psi_+(0) - \psi_-(0) = \lim_{\varepsilon \to 0} \int_{-\varepsilon}^{\varepsilon} \frac{d\psi}{dx} \, dx = 0.
\]  

(2.125)

Using these boundary conditions, we readily get the following system of two linear equations,
\[ A + B = F, \quad ikF - (ikA - ikB) = \frac{2m\omega}{\hbar^2} F, \]  
whose solution yields

\[ \frac{B}{A} = \frac{-i\alpha}{1 + i\alpha}, \quad \frac{F}{A} = \frac{1}{1 + i\alpha}, \quad \text{where} \quad \alpha = \frac{m\omega}{\hbar^2}. \]

(2.127)

For the barrier transparency \( T \equiv |F/A|^2 \), this result again gives Eq. (120). That formula may be recast to give a simple expression (valid only for \( E \ll U_{\text{max}} \)) for the transmission coefficient,

\[ T = \frac{1}{1 + \alpha^2} = \frac{E}{E + E_0}, \quad \text{where} \quad E_0 = \frac{m\omega^2}{2\hbar^2}, \]

(2.128)

that shows that as energy becomes larger than parameter \( E_0 \), the barrier’s transparency approaches unity.

However, the most important application of Eqs. (126) is for deriving transparency of more complex potential profiles. For that, let us first introduce very general notions of the scattering and transfer matrices, currently for the 1D case. Consider an arbitrary but finite-length potential “bump” (more formally called a scatterer), localized somewhere between points \( x_1 \) and \( x_2 \), on the flat potential background, say \( U = 0 \) (Fig. 13). We know the general solution, with a certain energy \( E \), outside the interval are a set of two sinusoidal waves. Let us present them in the form

\[ \psi_j = A_j e^{ik(x-x_j)} + B_j e^{-ik(x-x_j)}, \]

(2.129)

where (for now) \( j = 1 \) or 2, and \( \hbar k^2 / 2m = E \). Note that each of the wave pairs (129) has, in this notation, its own reference point \( x_j \), because this is very convenient for the calculations which follow.

As we have already discussed, if the wave/particle is incident from the left, the linear Schrödinger equation within the scatterer range \( x_1 < x < x_2 \), can provide only linear expressions of the transmitted \( (A_2) \) and reflected \( (B_1) \) wave amplitudes via the incident wave amplitude \( A_1 \):

\[ A_2 = S_{21}A_1, \quad B_1 = S_{11}A_1, \]

(2.130)

where \( S_{11} \) and \( S_{21} \) are certain (generally, complex) coefficients. In this case, \( B_2 = 0 \). Alternatively, if a wave, with amplitude \( B_2 \), is incident from the right, it also may induce a transmitted wave \( (B_1) \) and reflected wave \( (A_2) \) with amplitudes

\[ B_1 = S_{12}B_2, \quad A_2 = S_{22}B_2, \]

(2.131)

where coefficients \( S_{22} \) and \( S_{12} \) are generally different from \( S_{11} \) and \( S_{21} \). Now we can use the linear superposition principle to argue that if waves \( A_1 \) and \( B_2 \) are simultaneously incident on the scatterer (say,
because wave $B_2$ has been partly reflected back by some other scatterer located at $x > x_2$), the resulting scattered wave amplitudes $A_2$ and $B_1$ are just the sums of their values for separate incident waves:

$$B_1 = S_{11}A_1 + S_{12}B_2,$$
$$A_2 = S_{21}A_1 + S_{22}B_2.$$  \(2.132\)

These linear relations may be conveniently presented by the so-called scattering matrix (frequently called just “S-matrix”):

$$\begin{pmatrix} B_1 \\ A_2 \end{pmatrix} = S \begin{pmatrix} A_1 \\ B_2 \end{pmatrix},$$
$$S \equiv \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}.$$  \(2.133\)

Scattering matrices, duly generalized, are an important tool for the analysis of wave scattering in more than one dimensions; for 1D problems, however, another matrix is more convenient to present the same linear relations (132). Indeed, let us solve this system for $A_2$ and $B_2$. The result is

$$A_2 = T_{11}A_1 + T_{12}B_1,$$
$$B_2 = T_{21}A_1 + T_{22}B_1,$$

i.e.

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = T \begin{pmatrix} A_1 \\ B_1 \end{pmatrix},$$  \(2.134\)

where $T$ is the transfer matrix with elements

$$T_{11} = S_{21} - \frac{S_{11}S_{22}}{S_{12}}, \quad T_{12} = \frac{S_{22}}{S_{12}}, \quad T_{21} = -\frac{S_{11}}{S_{21}}, \quad T_{22} = \frac{1}{S_{12}}.$$  \(2.135\)

One can wonder whether matrices $S$ and $T$ obey any universal properties that would be valid for an arbitrary (but time-independent) scatterer. Such universal equations may be readily found from the probability current conservation and the time-reversal symmetry of the Schrödinger equation. Let me leave finding these relations for reader’s exercise. The results show, in particular, that the scattering matrix may be rewritten in the following form:

$$S = e^{i\theta} \begin{pmatrix} r e^{i\varphi} & t \\ t & -r e^{-i\varphi} \end{pmatrix},$$  \(2.136a\)

where 4 real parameters $r$, $t$, $\theta$, and $\varphi$ satisfy just one universal relation:

$$r^2 + t^2 = 1.$$  \(2.136b\)

(so that only 3 of the parameters are independent). As a result of this symmetry, $T_{11}$ may be also presented in a simpler form, similar to $T_{22}$: $T_{11} = \exp \{i\theta\}/t = 1/S_{12} = 1/S_{21}^*$. The last form allows a ready expression of scatterer’s transparency via just one coefficient of the transfer matrix:

$$T \equiv \left| \frac{A_2}{A_1} \right|^2 = \left| \frac{A_2}{B_2} \right|^2 = \left| \frac{S_{21}}{S_{12}} \right|^2 = \left| T_{11} \right|^2.$$  \(2.137\)

In our current context, the most important property of 1D transfer matrices is that in order to find the total transfer matrix $T$ of a system consisting of several (say, $N$) sequential arbitrary scatterers (Fig. 14), it is sufficient to multiply their matrices. Indeed, extending the definition (134) to other points $x_j$ ($j = 1, 2, \ldots, N+1$), we can write
\[
\begin{pmatrix}
A_2 \\
B_2
\end{pmatrix} = T_1 \begin{pmatrix}
A_1 \\
B_1
\end{pmatrix}, \quad \begin{pmatrix}
A_3 \\
B_3
\end{pmatrix} = T_2 \begin{pmatrix}
A_2 \\
B_2
\end{pmatrix} = T_2 T_1 \begin{pmatrix}
A_1 \\
B_1
\end{pmatrix},
\] (2.138)

etc. (where the matrix indices indicate the scatterers’ order on axis \(x\)), so that

\[
\begin{pmatrix}
A_{N+1} \\
B_{N+1}
\end{pmatrix} = T_N T_{N-1} \ldots T_1 \begin{pmatrix}
A_1 \\
B_1
\end{pmatrix},
\] (2.139)

But we can also define the total transfer matrix similarly to Eq. (134), i.e. as

\[
\begin{pmatrix}
A_{N+1} \\
B_{N+1}
\end{pmatrix} \equiv T \begin{pmatrix}
A_1 \\
B_1
\end{pmatrix},
\] (2.140)

so that finally

\[
T = T_N T_{N-1} \ldots T_1.
\] (2.141)

This formula is valid even if the flat-potential gaps between component scatterers vanish, so that it may be applied to a scatterer with an arbitrary profile \(U(x)\), by fragmenting its length into small segments \(\Delta x = x_{j+1} - x_j\), and treating each fragment as a rectangular barrier of height \((U_j)_{ef} = [U(x_{j+1}) - U(x_j)]/2\) - see Fig. 15. Since very efficient numerical algorithms are readily available for fast multiplication of matrices (especially as small as 2×2), this approach is broadly used in practice for the computation of transparency of tunnel barriers with complicated profiles \(U(x)\). (This is much more efficient than the direct numerical solution of the Schrödinger equation.)

In order to use this approach for several conceptually important systems, let us calculate the transfer matrices for a few elementary scatterers, starting from the delta-functional barrier located at \(x = 0\). Taking \(x_1 = x_2 = 0\), we can merely change the notation of wave amplitudes in Eq. (127) to get
An absolutely similar analysis of the wave incidence from the left yields
\[ S_{21} = \frac{-i\alpha}{1+i\alpha}, \quad S_{22} = \frac{1}{1+i\alpha}, \quad (2.142b) \]
and using Eqs. (135), we get
\[ T_\alpha = \begin{pmatrix} 1 - i\alpha & -i\alpha \\ i\alpha & 1 + i\alpha \end{pmatrix}. \quad (2.143) \]

The next example may seem strange at the first glance: what if there is no scatterer at all between points \( x_1 \) and \( x_2 \)? If points \( x_1 \) and \( x_2 \) coincide, the answer is indeed trivial and can be obtained, e.g., from Eq. (143) by taking \( W = 0 \), i.e. \( \alpha = 0 \):
\[ T_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \equiv I \quad (2.144) \]
- the so-called identity matrix. However, we are free to choose the reference points \( x_{1,2} \) participating in Eq. (129) as we wish. For example, what if \( x_2 - x_1 = a \)? Let us first take the forward-propagating wave alone: \( B_2 = 0 \) (and hence \( B_1 = 0 \)); then
\[ \psi_2 = \psi_1 = A_1 e^{ik(x-x_1)} = A_1 e^{ik(x_2-x_1)} e^{ikx_1} \quad (2.145) \]
Comparison of this expression with the definition (129) for \( j = 2 \) shows that \( A_2 = A_1 \exp\{ik(x_2-x_1)\} = A_1 \exp\{ika\} \), i.e. \( T_{11} = \exp\{ika\} \). Repeating the calculation for the back-propagating wave, we see that \( T_{22} = \exp\{-ika\} \), and since this “no-potential” (space interval) provides no particle reflection, we finally get
\[ T_\alpha = \begin{pmatrix} e^{ika} & 0 \\ 0 & e^{-ika} \end{pmatrix}, \quad (2.146) \]
independently of the mutual position of points \( x_1 \) and \( x_2 \). At \( a = 0 \), we naturally recover the special case (143).

Now let us use these results to analyze the double-barrier system shown in Fig. 16. We could of course calculate its properties as before, writing down explicit expressions for all 5 traveling waves shown by arrows in Fig. 16, and then using boundary conditions (124) and (125) at each of points \( x_{1,2} \) to get a system of 4 linear equations, and then solving it for 4 amplitude ratios.
However, the transfer matrix approach simplifies the calculations, because we may immediately use Eqs. (141), (143), and (146) to write

\[
T = T^a_a T^a T_a = \begin{pmatrix}
1-i\alpha & -i\alpha \\
i\alpha & 1+i\alpha
\end{pmatrix}
\begin{pmatrix}
e^{ika} & 0 \\
0 & e^{-ika}
\end{pmatrix}
\begin{pmatrix}
1-i\alpha & -i\alpha \\
i\alpha & 1+i\alpha
\end{pmatrix}
\]  
(2.147)

Let me hope that the reader remembers the “row by column” rule of the multiplication of square matrices;\(^{33}\) using it for two last matrices, we reduce Eq. (147) to

\[
T = \begin{pmatrix}
1-i\alpha & -i\alpha \\
i\alpha & 1+i\alpha
\end{pmatrix}
\begin{pmatrix}
(1-i\alpha)e^{ika} & -i\alpha e^{ika} \\
i\alpha e^{-ika} & (1+i\alpha)e^{-ika}
\end{pmatrix}
\]  
(2.148)

Now there is no need to calculate all elements of the full product \(T\), because, according to Eq. (137), for the calculation of barrier transparency \(T\) we need only one its element, \(T_{11}\):

\[
T = \frac{1}{|T_{11}|^2} = \frac{1}{\alpha^2 e^{-ika} + (1-i\alpha)^2 e^{ika}}
\]  
(2.149)

This result is similar to that following from Eq. (79) for \(E > U_0\): the transparency is a \(\pi\)-periodic function of the product \(ka\), reaching the maximum \((T = 1)\) at some point of each period – see Fig. 17a.

![Fig. 2.17. Resonant tunneling through a quantum well with delta-functional walls: (a) transparency a function of \(ka\), and (b) calculating resonance’s FWHM at \(\alpha >> 1\).](image)

However, the new result is different in that for \(\alpha >> 1\), the resonance peaks of transparency are very narrow, reaching their maxima at \(ka \approx k_n a \equiv n\pi\), with \(n = 1, 2, \ldots\) Physics of this effect is immediately clear from the comparison of this result with our analysis of the simplest quantum well – see Fig. 1.7 and its discussion. At \(k \approx k_n\), the incident wave, which undertakes multiple sequential reflections from the semi-transparent walls of the well, forms a nearly standing wave, which at \(\alpha >> 1\) virtually coincides with one of eigenfunctions of the well with infinite walls, with the standing wave amplitude much larger that that of the incident wave. As a result, the transmitted wave amplitude is

\[^{33}\text{In the analytical form: } (AB)_{ji} = \sum_{j'=1}^{N} A_{ji'}B_{j'i}, \text{ where } N \text{ is the matrix rank (in our current case, } N = 2).\]
proportionately increased. This is the famous effect of resonant tunneling\[^{34}\] in mathematical description identical to the resonant transmission of light through an optical \textit{Fabry-Perot resonator} formed by two parallel semi-transparent mirrors\[^{35}\].

Probably, the most surprising feature of this system is the fact that its maximum transparency is \textit{perfect} \((T_{\text{max}} = 1)\) even at \(\alpha \to \infty\), i.e. in the case of a very \textit{low} transparency of each of two component barriers\[^{36}\]. Indeed, the denominator in Eq. (149) may be interpreted as the squared length of the difference between two vectors, one of length \(\alpha^2\), and another of length \(|(1 - i\alpha)^2| = 1 + \alpha^2\), with angle \(\theta = 2ka + \text{const}\) between them. At the resonance, the vectors are aligned, and the difference is smallest (equal to 1) – see Fig. 17b, so that \(T_{\text{max}} = 1\).

We can use the same vector diagram to calculate the so-called FWHM, the common acronym for the \textit{Full Width [of the resonance curve at] Half-Maximum}, i.e. the difference \(\Delta k = k_+ - k\) between such two points on the opposite slopes of the same resonance, at which \(T = T_{\text{max}}/2\) - see arrows in Fig. 17a. Let the vectors in Fig. 17b be slightly misaligned, by an angle \(\theta \sim 1/\alpha^2 << 1\), so that the length of the difference vector (of the order of \(\alpha^2\theta\sim 1\)) is still much smaller than the length of each vector. In order to double its length squared, and hence reduce \(T\) by a factor of 2 in comparison with its maximum value 1, the arc, \(\alpha^2\theta\), between the vectors should also become equal \(\pm 1\), i.e. \(\alpha^2(2k_+a + \text{const}) = \pm 1\). Subtracting these two equations from each other, we finally get
\[
\Delta k \equiv (k_+ - k_-) = \frac{1}{a\alpha^2} \ll k_+ .
\]

Now let us use the simple potential shown in Fig. 16 to discuss an issue of large conceptual importance. For that, consider what would happen if at some initial moment (say, \(t = 0\)) we have placed a 1D quantum particle inside the double-barrier well with \(\alpha \gg 1\), and left it there alone, without any incident wave. To simplify the analysis, let us prepare the initial state so that it coincides with the ground state of the infinite-wall well – see Eq. (1.76):
\[
\Psi(x,0) = \psi_1(x) = \left(\frac{2}{a}\right)^{1/2} \sin[k_1(x - x_1)], \quad \text{where} \quad k_1 = \frac{\pi}{a} .
\]

At \(\alpha \to \infty\), this is an eigenstate of the system, and from our analysis in Sec. 1.5 we know its time evolution:
\[
\Psi(x,t) = \psi_1(x)e^{-i\omega t}, \quad \text{with} \quad \omega_1 = \frac{E_1}{\hbar} = \frac{\hbar k_1^2}{2m} = \frac{\hbar\pi^2}{2ma^2} ,
\]
telling us that the particle remains in the well at all times with constant probability \(W(t) = W(0) = 1\).\[^{37}\]

However, if parameter \(\alpha\) is large but finite, the de Broglie wave should slowly “leak out” from the well, so that \(W(t)\) would slowly decrease. Let us consider this effect approximately, assuming that

\[^{34}\] In older literature, it is sometimes called the \textit{Ramsauer} (or “Townsend”, or “Ramsauer-Townsend”) \textit{effect}. However, it is currently more common to use that name(s) only for a similar 3D effect, especially at scattering of low-energy electrons on rare gas atoms – this is how it was first observed, independently, by C. Ramsauer and J. Townsend in the early 1920s.

\[^{35}\] See also, e.g., EM Sec.7.9.

\[^{36}\] The exact equality \(T_{\text{max}} = 1\) is correct only if both component barriers are exactly equal.

\[^{37}\] Probability \(W(t)\) should not be confused with the delta-functional barrier’s “area” \(\mathcal{W}\), defined by Eq. (122).
the slow leakage, with a characteristic time \( \tau >> 1/\omega_1 \), does not affect the instant wave distribution inside the well, besides the reduction of \( W \). Then we can generalize Eqs. (151), (152) as follows:

\[
\Psi(x,t) = \left( \frac{2W}{a} \right)^{1/2} \sin[k_1(x-x_1)] e^{-i\omega_1 t}.
\]  

(2.153)

making the probability of finding the particle in the well equal to \( W \). This solution may be presented as a sum of two traveling waves:

\[
\Psi(x,t) = A e^{i(k_1 x - \omega_1 t)} + B e^{-i(k_1 x + \omega_1 t)},
\]  

(2.154)

with equal magnitudes of their amplitudes and probability currents

\[
|A| = |B| = \left( \frac{W}{2a} \right)^{1/2}, \quad I_A = \frac{\hbar}{m} |A|^2 k_1 = \frac{\hbar W}{m} \frac{\pi}{2a^2}, \quad I_B = -I_A.
\]  

(2.155)

But we already know from Eq. (128) that at \( \alpha >> 1 \) the delta-functional wall transparency \( T \) approximately equals \( 1/\alpha^2 \), so that the wave carrying current \( I_A \), incident on the right wall from inside, induces an outcoming waves outside of the well (Fig. 18) with the following probability current:

\[
I_R = \frac{1}{\alpha^2} I_A = \frac{1}{\alpha^2} \frac{\pi \hbar W}{2ma^2}.
\]  

(2.156a)

Absolutely similarly,

\[
I_L = \frac{1}{\alpha^2} I_B = -I_R.
\]  

(2.156b)

Fig. 2.18. Metastable state’s decay in the simple model of a 1D potential well with low-transparent walls – schematically.

Now we may combine the 1D version (6) of the probability conservation law for well’s interior,

\[
\frac{dW}{dt} + I_R - I_L = 0,
\]  

(2.157)

with Eqs. (156) to write

\[
\frac{dW}{dt} = -\frac{1}{\alpha^2} \frac{\pi \hbar}{ma^2} W.
\]  

(2.158)

---

38 This almost evident assumption finds its formal justification in the perturbation theory to be discussed in Chapter 6.
This is just the standard differential equation,
\[
\frac{dW}{dt} = -\frac{1}{\tau} W,
\]  
(2.159)
of the exponential decay, with solution \(W(t) = W(0)\exp\{-t/\tau\}\), where constant \(\tau\), in our case equal to
\[
\tau = \frac{ma^2}{\pi\hbar} \alpha^2,
\]  
(2.160)
is called the metastable state’s lifetime. Using expression (2.34) for the de Broglie waves’ group velocity, in our particular wave vector giving \(v_{gr} = \hbar k_{1}/m = \pi\hbar/ma\), Eq. (159) may be rewritten as
\[
\tau = \frac{t_A}{T},
\]  
(2.161)
where in our case the attempt time \(t_A\) is equal to \(a/v_{gr}\) and \(T = 1/\alpha^2\). Relation (161), that is valid for a large class of metastable systems,\(^{39}\) may be interpreted in the following semi-classical way. The confined particle travels back and forth between the confining walls, with time intervals \(t_A\) between the moments of incidence, each time making an attempt to leak through the wall, with a success probability of \(T\), so the reduction of \(W\) per each incidence is \(\Delta W = -WT\), immediately leading to Eq. (161).

Another important look at Eq. (160) may be taken by returning to the resonant tunneling problem and expressing the resonance width (150) in terms of incident particle’s energy:
\[
\Delta E = \Delta \left( \frac{\hbar^2 k^2}{2m} \right) \approx \frac{\hbar^2 k_1}{m} \Delta k = \frac{\hbar^2 k_1}{m} \frac{1}{a\alpha^2} = \frac{\pi\hbar^2}{ma^2 \alpha^2}.
\]  
(2.162)
Comparing Eqs. (160) and (162), we get a remarkably simple formula
\[
\Delta E \cdot \tau = \hbar.
\]  
(2.163)

This so-called energy-time uncertainty relation is certainly more general than our simple model; for example, it is valid for the lifetime and resonance tunneling width of any metastable state. This seems very natural, since because of the energy identification with frequency, \(E = \hbar\omega\), typical for quantum mechanics, Eq. (163) may be rewritten as \(\Delta\omega \cdot \tau = 1\) and seems to follow directly from the Fourier transform in time, just as the Heisenberg’s uncertainty relation (1.35) follows from the Fourier transform in space. In some cases, these two relations are indeed interchangeable; for example, Eq. (24) for the Gaussian wave packet width may be rewritten as \(\delta E \cdot \Delta t = \hbar\), where \(\delta E = \hbar (d\omega/dk)\delta k = \hbar v_{gr}\delta k\) is the r.m.s. spread of energies of monochromatic components of the packet, while \(\Delta t \equiv \delta x/v_{gr}\) is the time scale of the packet passage through a fixed observation point \(x\).

However, Eq. (163) it is much less general than Heisenberg’s uncertainty relation (1.35). Indeed, in non-relativistic quantum mechanics, Cartesian coordinates (say, \(x\)) of a particle, components of its momentum (say, \(p_x\)), and energy \(E\) are regular observables, presented by operators. In contract, time is treated as a \(c\)-number argument, and is not presented by an operator, so that Eq. (163) cannot be derived

\(^{39}\) Essentially the only requirement is to have the attempt time \(\Delta t_A\) to be much longer than the effective time (instanton time, see Sec. 5.3 below) of tunneling through the barrier. In the delta-functional approximation for the barrier, the latter time vanishes, so that this requirement is always fulfilled.
in such general assumptions as Eq. (1.35). Thus the time-energy uncertainty relation should be applied with great caution. Unfortunately, not everybody is so careful. One can find, for example, wrong claims that due to this relation, the energy dissipated by any system performing an elementary (single-bit) calculation during time interval \( \Delta t \) has to be larger than \( \hbar/\Delta t \). Another incorrect statement is that the energy of a system cannot be measured, during time \( \Delta t \), with an accuracy better than \( \hbar/\Delta t \).

Now let us use our simple model of metastable state’s decay for a preliminary discussion of one aspect of quantum measurements. Figure 18 shows (schematically) the traveling wave packets emitted by the quantum well after its initial state \((152)\) had been prepared at \( t = 0 \). At \( t \gg \tau \), the well becomes essentially empty \((W << 1)\), and the whole probability distribution is localized in two clearly separated wave packets of equal amplitudes, moving from away with speed \( v_{gr} \), each “carrying the particle away” with a probability of 50%. Now assume an experiment has detected the particle on the left side of the well. Though the formalisms suitable for a quantitative analysis of the detection process will not be discussed until Sec. 7.7, due to the wide separation of the packets, we may safely assume that the detection may be done without any actual physical effect on the counterpart wave packet. But if we know that the particle has been found on the left, there is no chance to find it on the right.

If we attributed the wavefunction to all stages of this particular experiment, this situation might be rather confusing. Indeed, this would mean that the wavefunction within the right packet should instantly turn into zero - the so-called wave packet reduction — a process that could not be described by either Schrödinger equation or any other law of physics. However, if (as was already discussed in Sec. 1.3) we attribute the wavefunction to a statistical ensemble of similar experiments, there is no paradox here at all. While the two-packet picture we have calculated (Fig. 18) describes the full initial ensemble (regardless of the particle detection results), the “reduced packet” picture (with no wave packet on the right of the well) describes only a sub-ensemble of experiments with the particle detected on the left side. As was discussed on completely classical examples in Sec. 1.3, for such sub-ensemble the probability distribution, and hence the wavefunction, may be dramatically different.

2.6. Coupled quantum wells

Let us now move on to tunneling through a more complex potential profile shown in Fig. 19: a sequence of \((N-1)\) similar quantum wells separated by \( N \) similar delta-functional tunnel barriers. According to Eq. (141), its transfer matrix is the following product

\[
T = T_a T_a T_a \ldots T_a T_a ,
\]

with the component matrices given by Eqs. (143) and (146), and the barrier height parameter \( \alpha \) defined by the last of Eqs. (127).

---

40 Here I dare to refer the reader to my own old work K. Likharev, *Int. J. Theor. Phys.* 21, 311 (1982) that presented a constructive proof that at reversible computation (introduced in 1973 by C. Bennett) the energy dissipation may be lower than this apparent “quantum limit”.


42 This argument is especially convincing if the particle detection time is much shorter than the time \( t_c = 2v_{gr}l/c \), where \( c \) is the speed of light in vacuum, i.e. the maximum velocity of any information transfer (“signaling”).
Remarkably, this multiplication may be carried out analytically, giving

\[ T \equiv |T_{11}|^2 = \left( \cos Nqa \right)^2 + \left( \frac{\sin ka - \alpha \cos ka}{\sin qa} \sin Nqa \right)^2 \] \quad \text{(2.165)}

where \( q \) is a new parameter, with the wave number dimensionality, defined by the following relation:

\[ \cos qa \equiv \cos ka + \alpha \sin ka. \] \quad \text{(2.166)}

For \( N = 1 \), Eqs. (165) and (166) immediately yield our old result (128), while for \( N = 2 \) they may be reduced to Eq. (149) – see Fig. 17a. Figure 20 shows its predictions for two larger numbers \( N \), and several values of parameter \( \alpha \).

Let us start discussion of the plots from case \( N = 3 \), i.e. two coupled quantum wells. The comparison of Fig. 20a and Fig. 17a shows that the transmission patterns, and their dependence on parameter \( \alpha \), are very similar, besides that in the coupled wells each resonant tunneling peak splits into two, with the \( ka \)-difference between them scaling as \( 1/\alpha \). In order to comprehend the physics of this important result, let us analyze an auxiliary system shown in Fig. 21: two similar quantum wells

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43 This formula will be easier to prove after we have discussed properties of Pauli matrices in Chapter 4.
confined by infinitely high potential walls at \( x = \pm a \), and coupled via a transparent, short tunnel barrier at \( x = 0 \).

The barrier may be again, for calculation simplicity, approximated by a delta-function:

\[
U(x) = \begin{cases} 
+ \infty, & \text{for } |x| > a, \\
\mathcal{W}, & \text{for } |x| < a.
\end{cases}
\] (2.167)

We already know that the standing-wave eigenfunctions \( \psi_n \) of the Schrödinger equation in regions with \( U(x) = 0 \), in our current case, segments \( -a < x < 0 \) and \( 0 < x < +a \), may be always presented as linear superpositions of \( \sin kx \) and \( \cos kx \). In order to immediately satisfy the boundary conditions \( \psi = 0 \) at \( x = \pm a \), we can take these solutions in the form

\[
\psi_s(x) = \begin{cases} 
C_- \sin k(x + a), & \text{for } -a < x < 0, \\
C_+ \sin k(x - a), & \text{for } 0 < x < +a.
\end{cases}
\] (2.168)

What remains is to satisfy the boundary conditions at \( x = 0 \). Plugging Eq. (167) into Eqs. (124) and (125), we get the following system of two linear equations:

\[
kaC_+C_mkaC_+C_mka = \cos k a,
\] (2.169)

\[
kaC_mC_+C_mkaC_+C_mka = \sin k a.
\] (2.170)

The system has two types of solutions, with the two lowest-energy eigenfunctions sketched in Fig. 21:

(i) **Antisymmetric solutions** (which will be marked with index \( A \)),

\[
(C_+)_A = (C_-)_A, \quad \text{i.e. } \psi_A = C_A \sin k_A x,
\] (2.171)

with eigenvalues independent of \( W \),

\[
\sin k_A a = 0, \quad \text{i.e. } k_A a = k_n a \equiv n, \quad n = 1, 2, ...
\] (2.172)

Notice that these values of \( k \), and hence eigenenergies of these antisymmetric states,

\[
E_A = \frac{\hbar^2 k_A^2}{2m} \equiv \frac{\pi^2 n^2}{2ma^2},
\] (2.173)
coincide with those of the simple quantum well of width $a$ – see Fig. 1.7 and its discussion.

(ii) **Symmetric solutions** (index $S$):

$$
(C_+)_S = - (C_-)_S, \quad \text{i.e.} \quad \psi_s = C_s \sin k_s (x - a),
$$

with Eq. (169) giving the following *characteristic equation* for constant $k_S$:

$$
\tan k_s a = - \frac{1}{\alpha}.
$$

Figure 22 shows the graphic solution of this equation for three values of parameter $\alpha$, i.e. for various quantum well coupling strength. For each solution, $k_S a$ is confined within interval

$$
\pi n < k_s a < \pi n - \frac{\pi}{2},
$$

so that the antisymmetric and symmetric states alternate on the scale of $k$ (and hence of the energy), with the difference $k_A - k_S$, for each pair of adjacent states, smaller then $\pi/2a$ for any value of $\alpha$. The physics of the splitting between eigenenergies corresponding to the symmetric and antisymmetric states is very simple: it is the change of kinetic energy of the particle due to different confinement types – see Fig. 21. In each antisymmetric mode, $\psi_n (0) = \psi_n (\pm a) = 0$, i.e. the wavefunction is essentially confined within a segment of length $a$; as a result, its energy (173) does not depend on the barrier height. On the contrary, in the symmetric mode, that does engage the potential barrier, the wavefunction effectively spreads into the counterpart well. As a result, it changes slower, and hence its kinetic energy is also lower than that of the adjacent antisymmetric mode.

By the way, this problem may serve as a toy model of the strongest (and most important) type of atom cohesion - the *covalent* (or “chemical”) bonding in molecules, liquids, and solids. The classical example of such bonding is that of hydrogen atoms in a H$_2$ molecule.$^{44}$ Each of two electrons of this system$^{45}$ reduces its kinetic energy very substantially by spreading its wavefunction around both nuclei

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44 Historically, the development of the fully quantum theory of H$_2$ bonding by W. Heitler and F. London in 1927 was the breakthrough decisive for the acceptance of then-emerging quantum mechanics by chemists.

45 Due to the opposite spins, the Pauli principle allows them to be in the same orbital ground state – see Chapter 8.
protons, rather than being confined near one of them - as it had to be in a single atom. As a result, the bonding is very strong: in chemical units, 429 kJ/mol, i.e. 18.6 eV per molecule.\(^\text{46}\) Somewhat counter-intuitive, this energy is substantially larger than the strongest classical (ionic) bonding due to electron transfer between atoms, leading to the Coulomb attraction of the resulting ions. (For example, the atomic cohesion in the NaCl molecule is just 3.28 eV.)

In the limit \(\alpha \to 0\) (no partition between the wells), \(k_S a \to \pi(n - 1/2)\), i.e. the eigenstates approach the shape and energy of symmetric states of a quantum well of width \(2a\). In the opposite limit \(\alpha \gg 1\), \(k_S a \to \pi n\), and in the vicinity of each such point we may approximate \(\tan k_S a\) with \((k_S a - \pi n)\) – see the dashed line in Fig. 22. As a result, the characteristic equation (175) is reduced to

\[
\alpha \pi = \frac{1}{\alpha a},
\]

so that the splitting between the wave numbers and eigenenergies of the adjacent symmetric and antisymmetric states is small:

\[
k_A - k_S \approx \frac{1}{\alpha a} \ll k_n, \quad 2\delta_n \equiv E_A - E_S \approx \frac{dE}{dk} (k_A - k_S) = \frac{\pi n\hbar^2}{ma} \frac{1}{\alpha a} = \frac{2E_A}{\pi n a}.
\]

(By construction, this result is valid only if \(\alpha \gg 1\), i.e. \(\delta_n \ll E_A \approx E_S\).)

Let us analyze properties of the system in this limit in much more detail - first, because the results will help us to develop the important tight binding approximation in the band theory, and second, because the weakly coupled quantum wells will be our first example of very important two-level (or “spin-½-like”) systems. Let us focus on one couple of symmetric and antisymmetric states, corresponding to virtually the same \(E_n\). According to Eqs. (171) and (174), in the limit \(\alpha \to \infty\), system’s eigenfunctions may be approximately represented as follows:

\[
\psi_S(x) \approx \frac{1}{\sqrt{2}} [\psi_R(x) + \psi_L(x)] \quad \psi_A(x) = \frac{1}{\sqrt{2}} [\psi_R(x) - \psi_L(x)],
\]

where \(\psi_{R,L}\) are the normalized ground states of the completely insulated wells:

\[
\psi_R(x) = \begin{cases} 
0, & \text{for } -a < x < 0, \\
\left(\frac{2}{a}\right)^{1/2} \sin k_n x, & \text{for } 0 < x < +a,
\end{cases} \quad \psi_L(x) = \begin{cases} 
-(2/a)^{1/2} \sin k_n x, & \text{for } -a < x < 0, \\
0, & \text{for } 0 < x < +a.
\end{cases}
\]

Let us perform the following conceptually important thought experiment: place the particle, at \(t = 0\), into one of the localized states, say \(\psi_R(x)\), and leave the system alone to evolve. Solving Eqs (180) for \(\psi_R\), we may present the initial state as a linear superposition of eigenfunctions:

\[
\Psi(x,0) = \psi_R(x) \approx \frac{1}{\sqrt{2}} [\psi_S(x) + \psi_A(x)].
\]

Now, according to the general solution (1.67) of the time-independent Schrödinger equation, time dynamics may be obtained by just multiplying each eigenfunction by the corresponding factor (1.61):
\[ \Psi(x,t) = \frac{1}{\sqrt{2}} \left[ \psi_S(x) \exp \left\{ -i \frac{E_S}{\hbar} t \right\} + \psi_A(x) \exp \left\{ -i \frac{E_A - E_S}{\hbar} t \right\} \right]. \]

Now, introducing the following natural notation,

\[ E_n \equiv \frac{E_A + E_S}{2}, \quad \delta_n \equiv \frac{E_A - E_S}{2}. \]  

And using Eqs. (179), this expression may be rewritten as

\[ \Psi(x,t) = \frac{1}{\sqrt{2}} \left[ \psi_S(x) \exp \left\{ i \frac{\delta_n}{\hbar} t \right\} + \psi_A(x) \exp \left\{ -i \frac{\delta_n}{\hbar} t \right\} \right] \exp \left\{ -i \frac{E_n}{\hbar} t \right\} \]

\[ = \left[ \psi_R(x) \cos \frac{\delta_n}{\hbar} t + i \psi_I(x) \sin \frac{\delta_n}{\hbar} t \right] \exp \left\{ -i \frac{E_n}{\hbar} t \right\}. \]  

This result implies, in particular, that the probabilities \( W_R \) and \( W_L \) to find the particle, correspondingly, in the right and left wells change with time as

\[ W_R = \cos^2 \frac{\delta_n}{\hbar} t, \quad W_L = \sin^2 \frac{\delta_n}{\hbar} t, \]  

mercifully leaving the total probability constant \( W_R + W_L = 1 \). (If our calculation had not passed this sanity check, we would be in a big trouble.)

This is the famous effect of periodic quantum oscillations, with frequency \( \omega_n = 2\delta_n/\hbar = (E_A - E_S)/\hbar \), of the particle between two similar quantum wells, due to their coupling through via tunneling through the tunnel barrier. The physics of this effect is straightforward: just as in the single well problem discussed in Sec. 5, the particle initially placed into a certain quantum well tries to escape from it via tunneling through the semi-transparent wall. However, in our current situation (Fig. 21) the particle can only escape into the adjacent well. After the tunneling into that second well, the tries to escape from it, and hence comes back, etc. - just as a classical 1D oscillator, initially deflected from its equilibrium position.

Maybe the most surprising feature of this effect is its relatively high frequency: according to Eq. (178), the time period of the quantum oscillations,

\[ \Delta t_n \equiv \frac{2\pi}{\omega_n} = \frac{2\pi \hbar}{(E_A - E_S)} \approx \frac{2\pi}{n} \frac{m a^2}{\hbar}, \quad \text{for } \alpha >> 1, \]  

is a factor of \( \alpha/2\pi >> 1 \) shorter than the lifetime \( \tau \) (160) of the metastable state of the particle in a similar but single quantum well limited by delta-functional walls with similar parameter \( \alpha \). This is a very counterintuitive result indeed: the speed of particle tunneling into a similar adjacent well is much higher than that, through a similar barrier, to the free space!

To see whether this result is an artifact of the delta-functional model of the tunnel barrier, let us calculate splitting \( 2\delta_n \) for system of two similar, symmetric, soft quantum wells formed by a smooth potential profile \( U(x) = U(-x) \) – see Fig. 23.
If the barrier transparency is low, the quasi-localized wavefunctions \( \psi_R(x) \) and \( \psi_L(x) = \psi_R(-x) \) and their eigenenergies may be found approximately by solving the Schrödinger equations in one of the wells, neglecting tunneling through the barrier, but finding \( \delta_n \) requires a little bit more care. Let us write the stationary Schrödinger equations for the symmetric and antisymmetric solutions in the form

\[
\begin{align*}
\left[ E_A - U(x) \right] \psi_A &= -\frac{\hbar^2}{2m} \frac{d^2 \psi_A}{dx^2}, \\
\left[ E_S - U(x) \right] \psi_S &= -\frac{\hbar^2}{2m} \frac{d^2 \psi_S}{dx^2},
\end{align*}
\]

then multiply the former equation by \( \psi_S \), the latter one by \( \psi_A \), subtract them from each other, and integrate the result from 0 to \( \infty \):

\[
(E_A - E_S) \int_0^\infty \psi_S \psi_A dx = \frac{\hbar^2}{2m} \int_0^\infty \left[ \frac{d^2 \psi_S}{dx^2} \psi_A - \frac{d^2 \psi_A}{dx^2} \psi_S \right] dx. \tag{2.188}
\]

If \( U(x) \), and hence \( \frac{d^2 \psi_A, S}{dx^2} \), are finite for all \( x \),\(^{47}\) we may integrate the right-hand side by parts to get

\[
(E_A - E_S) \int_0^\infty \psi_S \psi_A dx = \frac{\hbar^2}{2m} \left[ \frac{d \psi_S}{dx} \psi_A - \frac{d \psi_A}{dx} \psi_S \right]_0^\infty. \tag{2.189}
\]

So far, this is an exact equation. For weakly coupled wells, we can do more. In this case, the left hand side may be approximated as \( (E_A - E_S)/2 = \delta_n \), because the integral is dominated by the vicinity of point \( a \), where the second terms in each of Eqs. (179) are negligible, and the integral is equal to ½, due to the proper normalization of function \( \psi_R(x) \). In the right-hand side, the substitution at \( x = \infty \) vanishes (due to the wavefunction decay in the classically forbidden region), and so does the first term at \( x = 0 \), because for the antisymmetric solution \( \psi_A(0) = 0 \). As a result, we get

\[
\delta_n = \frac{\hbar^2}{2m} \psi_S(0) \frac{d \psi_A}{dx}(0) = \frac{\hbar^2}{m} \psi_R(0) \frac{d \psi_R}{dx}(0) = \frac{\hbar^2}{m} \psi_L(0) \frac{d \psi_L}{dx}(0) = \frac{\hbar^2}{m} \psi_L(0) \frac{d \psi_L}{dx}(0). \tag{2.190}
\]

It is straightforward to show that within the limits of the WKB approximation validity, Eq. (190) may be reduced to

\[
\delta_n = \frac{\hbar}{t_A} \exp \left\{ -\int_{x_c}^{x_e} \kappa(x') dx' \right\}. \tag{2.191}
\]

\(^{47}\) Since it is not true for potential (167), one should not be surprised that the resulting Eq. (189) is invalid for our initial problem, giving \( \delta_n \) twice larger than the correct expression (178).
where \( t_A \) is the time period of classical motion of the particle inside one of the wells, function \( \alpha(x) \) is defined by Eq. (97), and \( x_c \) and \( x_c' \) are the classical turning points limiting the potential barrier at the level \( E_n \) of particle’s energy – see Fig. 23. Comparing this result with Eq. (117), we can notice that again, just as in the case of the delta-functional barriers, the transmission coefficient \( T \) of a tunnel barrier (and hence the reciprocal lifetime of a metastable state in a potential well separated by such a barrier from a continuum) scales as the square of the WKB exponent participating in Eq. (191), so that the period of quantum oscillations between the well is much smaller than the lifetime. We will return to the discussion of this result, in a more general form, in Chapter 5.

Returning for a second to Fig. 20a, we may now readily interpret the results for tunneling through the double quantum well: each pair of resonance peaks of transparency corresponds to the alignment of incident particle’s energy with the pair of energy levels \( E_A, E_S \) of the symmetric and antisymmetric states of the system.

2.7. 1D band theory

Let us now return to Eqs. (165) and (166) describing the resonant tunneling, and discuss their predictions for larger \( N \) – see, for example, Fig. 20b. We see that the increase of \( N \) results in the increase of the number of resonant peaks per period to \((N - 1)\), and at \( N \rightarrow \infty \) the peaks merge into the so-called allowed energy bands (frequently called just the “energy bands”) of relatively high transparency, separated from similar bands in the adjacent periods of function \( T(ka) \) by energy gaps\(^{48}\) where \( T \rightarrow 0 \). Notice the following important features of the pattern:

(i) at \( N \rightarrow \infty \), the band/gap edges become sharp for any \( \alpha \), and tend to fixed positions (determined by \( \alpha \) but independent of \( N \));

(ii) the larger interwell coupling \((\alpha \rightarrow 0)\), the broader the allowed energy bands and narrower the gaps between them.

Our discussion of resonant tunneling in the previous section gives us an evident clue for a semi-quantitative interpretation of this pattern: if \((N - 1)\) quantum wells are weakly coupled by tunneling through the tunnel barriers separating them, system’s energy spectrum consists of groups \((N - 1)\) energy levels. Each level corresponds to an eigenfunction that is the set of similar local functions in each well, but with certain phase shifts \( \Delta \varphi \) between them. It is natural to expect that, just as for 2 coupled wells \((N - 1 = 2)\), that at the upper level, \( \Delta \varphi = \pi \) (thus providing the highest confinement), with \( ka \rightarrow m \) at \( \alpha \rightarrow \infty \), while at the lowest level all \( \Delta \varphi = 0 \), providing the most loose confinement.\(^{49}\) However, what about \( \Delta \varphi \) for other levels?

Answers to all these questions are easy to get in the most important limit \( N \rightarrow \infty \), i.e. for periodic structures - which are, in particular, good 1D approximations for solid state crystals, whose samples may feature more than \( 10^{10} \) similar atoms or molecules in each direction of the crystal lattice. It is almost self-evident that at \( N \rightarrow \infty \), due to the translational invariance of \( U(x) \),

\[
U(x + a) = U(x),
\]

\(^{48}\) In solid state (especially semiconductor) physics and electronics, term bandgaps is more common.

\(^{49}\) This expectation is implicitly confirmed by Fig. 20: at \( \alpha \gg 1 \), the highest resonance peak in each group tends to \( ka = \pi m \), and the lowest peak also tend to a position independent of \( N \) (though dependent on \( \alpha \)).
the phase shift $\Delta \phi$ between local wavefunctions in all adjacent quantum wells should be the same for each period of the system, i.e.

$$\psi(x + a) = \psi(x)e^{i\Delta \phi}$$  \hspace{1cm} (2.193a)

for all $x$. (A reasonably fair classical image of $\Delta \phi$ is the geometric angle between similar objects - e.g., similar paper clips - attached at equal distances to a long, uniform rubber band. If the band’s ends are twisted, the twist is equally distributed between the structure’s periods, representing the constancy of $\Delta \phi$.\textsuperscript{50})

Equation (193a) is the (1D version of the) much-celebrated \textit{Bloch theorem}.\textsuperscript{51} Mathematical rigor aside,\textsuperscript{52} it is a virtually evident fact, because the particle’s density $w(x) = \psi^*(x)\psi(x)$, that has to be periodic in this $a$-periodic system, may be so only $\Delta \phi$ is constant. For what follows, it is more convenient to present the real number $\Delta \phi$ in the form $qa$ (there is no loss of generality here, because parameter $q$ may depend on $a$ as well as other parameters of the system), so that the Bloch theorem takes the form

$$\psi(x + a) = \psi(x)e^{iqa}.$$  \hspace{1cm} (2.193b)

The physical sense of parameter $q$ will be discussed in detail below; for now just note that according to Eq. (193b), an addition of $(2\pi/a)$ to it yields the same wavefunction; hence all observables have to be $(2\pi/a)$-periodic functions of $q$.\textsuperscript{53}

Now let us use the Bloch theorem to find eigenfunctions and eigenenergies for a particular, and probably the simplest periodic function $U(x)$: an infinite set of similar quantum wells separated by delta-functional tunnel barriers (Fig. 24).

\textsuperscript{50} I am ashamed to confess that, due to the lack of time, this was virtually the only “lecture demonstration” in my QM courses.

\textsuperscript{51} Named after F. Bloch who applied this concept to wave mechanics in 1929, i.e. very soon after its formulation. Admittedly, in mathematics, an equivalent statement, usually called the \textit{Floquet theorem}, has been known since at least 1883.

\textsuperscript{52} I will address this rigor in two steps. Later in this section, we will see that the function obeying Eq. (193) is indeed a solution of the Schrödinger equation. However, to save time/space, it will be better for us to postpone the proof that \textit{any} eigenfunction of the equation, with periodic boundary conditions, obeys the Bloch theorem, until Chapter 4. As a partial reward for the delay, that proof will be valid for an arbitrary spatial dimensionality.

\textsuperscript{53} Product $h\tilde{q}$, which has the dimensionality of momentum, is called either the \textit{quasi-momentum} or (especially in the solid state physics) the “crystal momentum” of the particle.
To start, consider two points separated by distance $a$: one of them, $x_j$, just left of position of one of the barriers, and another one, $x_{j+1}$, just left of the following barrier. Eigenfunctions in each of the points may be presented as linear superpositions of two simple waves $\exp\{\pm ikx\}$, and amplitudes of their components should be related by a $2\times 2$ transfer matrix $T$ of the potential fragment separating them. According to Eq. (141), this matrix may be found as the product of the matrix (146) of one interval $a$ and the matrix (143) of one barrier:

$$
\begin{pmatrix}
A_{j+1} \\
B_{j+1}
\end{pmatrix} = T_a T_\alpha \begin{pmatrix}
A_j \\
B_j
\end{pmatrix} = \begin{pmatrix}
e^{ika} & 0 \\
0 & e^{-ika}
\end{pmatrix} \begin{pmatrix}1-i\alpha & -i\alpha \\
i\alpha & 1+i\alpha\end{pmatrix} \begin{pmatrix}A_j \\
B_j
\end{pmatrix}.
$$

(2.194)

However, according to the Bloch theorem (193b), the component amplitudes should be also related as

$$
\begin{pmatrix}
A_{j+1} \\
B_{j+1}
\end{pmatrix} = e^{iqa} \begin{pmatrix}
A_j \\
B_j
\end{pmatrix} = \begin{pmatrix}e^{iqa} & 0 \\
0 & e^{iqa}\end{pmatrix} \begin{pmatrix}A_j \\
B_j
\end{pmatrix}.
$$

(2.195)

The condition of self-consistency of these two equations leads to the following characteristic equation:

$$
\begin{pmatrix}
e^{ika} & 0 \\
0 & e^{-ika}\end{pmatrix} \begin{pmatrix}1-i\alpha & -i\alpha \\
i\alpha & 1+i\alpha\end{pmatrix} - \begin{pmatrix}e^{iqa} & 0 \\
0 & e^{iqa}\end{pmatrix} = 0.
$$

(2.196)

In Sec. 5, we have already calculated the matrix product participating in this equation – see Eq. (148). Using it, we see that Eq. (196) is reduced to the same simple Eq. (166) that has already jumped at us from the solution of the different (resonant tunneling) problem. Let us explore that simple result in detail. First of all, the right hand part of Eq. (166) is a sinusoidal function of $ka$, with amplitude $(1 + \alpha^2)^{1/2}$ – see Fig. 25, while its left hand part is a sinusoidal function of $qa$ with amplitude 1.

As a result, within each period $\Delta(ka) = 2\pi$, the characteristic equation does not have a real solution for $q$ inside two intervals of $ka$ - and hence inside two intervals of energy $E = \hbar^2 k^2/2m$. (These intervals are exactly the energy gaps mentioned above, while the complementary intervals of $ka$ and $E$, where a real $q$ exists, are the allowed energy bands.) In contrast, parameter $q$ can take any real values, so it is more convenient to plot the eigenenergy $E = \hbar^2 k^2/2m$ as the function of $q$ (or, even more...
conveniently, $qa$ rather than $ka$.\footnote{Perhaps a more important reason for taking $q$ as the argument is that for motion in a general potential $U(x)$, particle’s momentum $\hbar k$ is not a constant of motion, while (according to the Bloch theorem), the quasi-momentum $\hbar q$ is.} While doing that, we need to recall that parameter $\alpha$, defined by the last of Eqs. (127), depends on wave vector $k$ as well, so that if we vary $q$ (and hence $k$), it is better to characterize the structure by a different, $k$-independent dimensionless parameter, for example

$$\beta \equiv (ka)\alpha = \frac{maw}{\hbar^2}, \quad (2.197)$$

so that Eq. (166) becomes

$$\cos qa = \cos ka + \beta \frac{\sin ka}{ka}. \quad (2.198)$$

Figure 26 shows the plots of $E$ and $k$, following from Eq. (198), for a particular, moderate value of parameter $\beta$. The band structure of the energy spectrum is apparent. Another evident feature is the $2\pi$-periodicity of the pattern, that we have already predicted from the general Bloch theorem arguments. (Due to this periodicity, the complete band/gap pattern may be studied on just one interval $-\pi \leq qa \leq + \pi$, called the 1\textsuperscript{st} Brillouin zone – the so-called reduced zone picture. For some applications, however, it is more convenient to use the extended zone picture with $-\infty \leq qa \leq +\infty$ - see, e.g., the next section.)

![Figure 2.26](image-url)
However, maybe the most surprising fact, clearly visible in Fig. 26, is that there is an infinite number of energy bands, with different energies \( E_n(q) \) for the same value of \( q \). Mathematically, it is evident from Eq. (198) – see also Fig. 25. Indeed, for each value of \( qa \) there are two solutions \( ka \) to this equation on each period \( \Delta (ka) = 2\pi \) - see also panel (a) in Fig. 26. Each of such solutions gives a different value of particle energy \( E = \hbar^2 k^2 / 2m \). A continuous set of similar solutions for various \( qa \) forms a particular energy band.

Since the band theory is one of the most vital results of quantum mechanics, it is important to understand the physics of these different solutions - and hence of the whole band picture. For that, let us explore analytically two different potential strength limits. An important advantage of this approach is that both analyses may be carried out for an arbitrary periodic potential \( U(x) \), rather than for the simplest model shown in Fig. 24.

(i) **Tight-binding approximation.** This approximation is sound when eigenenergy \( E_n \) is much lower than the height of the potential barriers separating the potential minima (serving as quantum wells) – see Fig. 27. As should be clear from our discussion in Sec. 6, the wavefunction is mostly localized in the classically allowed regions at points \( x_j \) of the potential energy minima - see the dashed lines in Fig. 27. Essentially the only role of coupling between these quantum well states (via tunneling through the separating barriers) is to establish certain phase shifts \( \varphi = qa \) between the pairs of adjacent quasi-localized wavefunction “lumps” \( u(x - x_j) \) and \( u(x - x_{j+1}) \).

To describe this effect quantitatively, let us first return to the problem of two coupled wells considered in Sec. 6, and recast result (184) as

\[
\Psi_n(x,t) = [a_R(t)\psi_R(x) + a_L(t)\psi_L(x)]\exp\left\{-i\frac{E_n}{\hbar}t\right\}, \tag{2.199}
\]

where functions \( a_R \) and \( a_L \) oscillate sinusoidally in time:

\[
a_R(t) = \cos\frac{\delta_n}{\hbar}t, \quad a_L(t) = i\sin\frac{\delta_n}{\hbar}t. \tag{2.200}
\]

This evolution satisfies the following system of two equations whose structure reminds Eq. (1.59):

\[
i\hbar\dot{a}_R = -\delta_n a_L, \quad i\hbar\dot{a}_L = -\delta_n a_R. \tag{2.201}
\]

Later in the course (in Chapter 6) we will prove that such equations are indeed valid, in the tight-binding approximation, for any system of two coupled quantum wells. These equations may be readily generalized to the case of many similar coupled wells. Here, in this case, instead of Eq. (199), we evidently should write
\[ \Psi_n(x,t) = \exp\left\{-\frac{i E_n}{\hbar} t\right\} \sum_j a_j(t) u_n(x - x_j), \]  

(2.202)

where \( E_n \) are the eigenenergies, and \( u_n \) the eigenfunctions of each isolated well. In the tight binding limit, only the adjacent wells are coupled, so that instead of Eq. (201) we should write an infinite system of similar equations

\[ i\hbar \dot{a}_j = -\delta_n a_{j-1} - \delta_n a_{j+1}, \]  

(2.203)

for each well number \( j \), where parameters \( \delta_n \) describe the coupling between two adjacent quantum wells. Repeating the calculation outlined in the end of Sec. 6 for our new situation, we get the result essentially similar to the last form of Eq. (190):

\[ \delta_n = \frac{\hbar^2}{m} u_n'(x_0) (a - x_0), \]  

(2.204)

where \( x_0 \) is the distance between the well bottom and the middle of the tunnel barrier on the right of it – see Fig. 27. The only substantial new feature of this expression in comparison with Eq. (190) is that the sign of \( \delta_n \) alternates with the level number \( n \): \( \delta_1 > 0, \delta_2 < 0, \delta_3 > 0, \) etc. Indeed, the number of “wiggles” (formally, zeros) of eigenfunctions \( u_n(x) \) of any potential well increases as \( n \) – see, e.g., Fig. 1.7,\(^{55} \) so that the difference of the exponential tails of the functions, sneaking under the left and right barriers limiting the well also alternates with \( n \).

The infinite system of ordinary differential equations (203) allows one to explore a large range of important problems (such as the spread of the wavefunction that was initially localized in one well, etc.), but our main task now is to find its stationary states, i.e. the solutions proportional to \( \exp\{-i(\varepsilon_n/\hbar)t\} \), where \( \varepsilon_n \) is a still unknown, \( q \)-dependent addition to the background energy \( E_n \) of \( n \)-th level. In order to satisfy the Bloch theorem (193) as well, such solution should have the form

\[ a_j(t) = a \exp\left\{i q x_j - i \frac{\varepsilon_n}{\hbar} t + \text{const}\right\}, \]  

(2.205)

where \( a \) is a constant. Plugging this solution into Eq. (203) and canceling the common exponent, we get

\[ E = E_n + \varepsilon_n = E_n - \delta_n \left( e^{-iqa} + e^{iqa} \right) = E_n - 2\delta_n \cos qa, \]  

(2.206)

so that in this approximation, the energy band width \( \Delta E_n \) (see Fig. 26b) equals \( 4|\delta_n| \).

Relation (206), whose validity is restricted to \( \delta_n \| E_n \) describes the particular lowest energy bands plotted in Fig. 26b reasonably well. (For larger \( \beta \), the agreement would be even better.) So, this calculation explains what the energy bands really are – in the tight binding limit they are best interpreted as isolated well’s energy levels \( E_n \), broadened into bands by the interwell interaction. Also, this result gives a clear proof that the energy band extremes correspond to \( qa = 2\pi l \) and \( qa = 2\pi(l + \frac{1}{2}) \), with integer \( l \). Finally, the sign alteration of the coupling coefficient \( \delta_n \) (204) with number \( n \) explains why the energy maxima of one band are aligned, on the \( qa \) axis, with energy minima of the adjacent bands.

\(^{55}\) Below, we will see several other examples of this behavior. This alternation rule is also in accordance with the Bohr-Sommerfeld quantization condition
(ii) **Weak-potential limit.** Surprisingly, the energy band structure is also compatible with a completely different physical picture that can be developed in the opposite limit. Let energy \( E \) be so high that the periodic potential \( U(x) \) may be treated as a small perturbation. Naively, we would have the parabolic dispersion relation between particle’s energy and momentum. However, if we are plotting energy as a function of \( q \) rather than \( k \), we need to add \( 2\pi l/a \), with arbitrary integer \( l \), to the argument. Let us show this by expanding all variables into the spatial Fourier series. For a periodic potential energy \( U(x) \) such an expansion is straightforward:\(^{56}\)

\[
U(x) = \sum_{l'} U_{l'} \exp\left\{-i \frac{2\pi}{a} l' \right\}, \tag{2.207}
\]

where the summation is over all integers \( l'' \), from \(-\infty \) to \(+\infty \). However, for the wavefunction we should show due respect to the Bloch theorem (193). To understand how to proceed, let us define another function

\[
u(x) \equiv \psi(x) e^{-iqx}, \tag{2.208}\]

and study its periodicity:

\[
u(x + a) = \psi(x + a) e^{-i(q(x+a))} = \psi(x) e^{-iqx} = u(x). \tag{2.209}\]

We see that the new function is \( a \)-periodic, and hence we can use Eqs. (208)-(209) to rewrite the Bloch theorem as

\[
\psi(x) = u(x) e^{iqx}, \text{ with } u(x + a) = u(x). \tag{2.210}\]

Now it is safe to expand the periodic function \( u(x) \) exactly as \( U(x) \):

\[
u(x) = \sum_{l'} u_{l'} \exp\left\{-i \frac{2\pi}{a} l' \right\}, \tag{2.211}\]

so that, according to the Bloch theorem,

\[
\psi(x) = e^{iqx} \sum_{l'} u_{l'} \exp\left\{-i \frac{2\pi}{a} l' \right\} = \sum_{l'} u_{l'} \exp\left\{i \left( q - \frac{2\pi}{a} l' \right) x \right\}. \tag{2.212}\]

The only nontrivial part of plugging this expression into the stationary Schrödinger equation (61) is the calculation of the product term, using expansions (207) and (211):

\[
U(x)\psi = \sum_{l', l''} U_{l'} u_{l''} \exp\left\{i \left( q - \frac{2\pi}{a} (l' + l'') x \right) \right\}. \tag{2.213}\]

At fixed \( l' \), we may change summation over \( l'' \) to that over \( l \equiv l' + l'' \) (so that \( l'' = l - l' \)), and write:

\[
U(x)\psi = \sum_{l'} \exp\left\{i \left( q - \frac{2\pi}{a} l \right) x \right\} \sum_{l''} u_{l'} U_{l''}. \tag{2.214}\]

---

\(^{56}\)The benefits of my unusual choice of the summation index \( l'' \) instead of, say, \( l \) will be clear in a few lines.
Now plugging Eqs. (212) (with index \( l' \) now replaced by \( l \)) and (214) into the stationary Schrödinger equation (61), and requiring the coefficients of each spatial exponent to match, we get an infinite system of linear equations for \( u_l \):\(^{57}\)

\[
\sum_{l'} U_{l-l'} u_{l'} = \left[ E - \frac{\hbar^2}{2m} \left( q - \frac{2\pi}{a} l \right)^2 \right] u_l.
\] (2.215)

So far, this system is an equivalent alternative to the initial Schrödinger equation – and, by the way, is very efficient for fast numerical calculations, for virtually any potential strength, though in systems with tight binding it may require taking into account a large number of harmonics \( u_l \). In the weak potential limit, i.e. if all the Fourier coefficients \( U_n \) are small,\(^ {58}\) we can complete all the calculation analytically.\(^ {59}\) Indeed, in the so-called 0\(^{th}\) approximation we can ignore all \( U_n \), so that in order to have at least one \( u_l \) different from 0, Eq. (215) requires that

\[
E \rightarrow E_l = \frac{\hbar^2}{2m} \left( q - \frac{2\pi l}{a} \right)^2.
\] (2.216)

(\( u_l \) itself should be obtained from the normalization condition). This result means that the dispersion relation \( E(q) \) has an infinite number of similar quadratic branches numbered by integer \( l \) – see Fig. 28.

![Fig. 2.28. 1D band picture in the weak potential case (\( \Delta_n \ll E^{(0)} \)). Shading shows the 1\(^{st}\) Brillouin zone.](image)

On any branch, the eigenfunction has just one Fourier coefficient, i.e. presents a monochromatic traveling wave

\[
\psi_l \rightarrow u_i e^{ikx} = u_l \exp \left\{ i \left( q \cdot \frac{2\pi l}{a} \right) x \right\}.
\] (2.217)

\(^{57}\) Note that we have essentially proved that the Bloch wavefunction (210) is indeed a solution of Eq. (61), provided that the quasi-momentum \( q \) is selected in a way to make the system of linear equation (215) compatible, i.e. is a solution of its characteristic equation – see, e.g., Eq. (223) below.

\(^{58}\) Besides the constant potential \( U_0 \) that, as we know from Sec. 2, may be included into energy in a trivial way, so that we may take \( U_0 = 0 \).

\(^{59}\) This method is so powerful that its multi-dimensional version is not much more complex than the 1D version described here – see, e.g., Sec. 3.2 in the classical textbook by J. M. Ziman, *Principles of the Theory of Solids*, 2\(^{nd}\) ed., Cambridge U. Press, 1979.
The definition of $E_l$ allows us to rewrite Eq. (215) in a more transparent form

$$
\sum_{l \neq l'} U_{l-l'} u_{l'} = (E - E_l) u_l,
$$

(2.218)

that may be formally solved for $u_l$:

$$
u_l = \frac{1}{E - E_l} \sum_{l \neq l'} U_{l-l'} u_{l'} \tag{2.219}
$$

If the Fourier coefficients $U_n$ are nonvanishing but small, this formula shows that wavefunctions do acquire other Fourier components (besides the main one, with the index corresponding to the branch number), but these additions are all small, besides narrow regions near the points $E_l = E_{l'}$ where two branches (216) of the dispersion relation $E(q)$, with some specific numbers $l$ and $l'$, cross. This happens when

$$
\left( q - \frac{2\pi l}{a} \right) \approx - \left( q - \frac{2\pi l'}{a} \right), \tag{2.220}
$$

i.e. at $q \approx q_m \equiv \pi n / a$ (with integer $m \equiv l + l'$)\(^{60}\) corresponding to

$$
E_l \approx E_{l'} \approx \frac{\hbar^2}{2ma^2} \left[ \pi(l + l') - 2\pi l \right]^2 = \frac{\pi^2 \hbar^2}{2ma^2} n^2 \equiv E^{(n)}, \tag{2.221}
$$

with integer $n \equiv l - l'$. (Equation (221) shows that index $n$ is just the number of the branch crossing on the energy scale – see Fig. 28.) In such a region, $E$ has to be close to both $E_l$ and $E_{l'}$, so that the denominator in just one of the infinite number of terms in Eq. (219) is very small, making the term substantial despite the smallness of $U_n$. Hence we can take into account only one term in each of the sums (written for $l$ and $l'$):

$$
U_n u_l = (E - E_l) u_l, \quad U_{-n} u_l = (E - E_{l'}) u_{l'}. \tag{2.222}
$$

Taking into account that for any real function $U(x)$ the Fourier coefficients in series (207) have to be related as $U_n = U^*_n$, Eq. (222) yields the following simple characteristic equation

$$
\begin{vmatrix}
E - E_l & -U_n \\
-U^*_n & E - E_{l'}
\end{vmatrix} = 0, \tag{2.223}
$$

with solution

$$
E_{\pm} = E_{\text{ave}} \pm \left[ \frac{(E_l - E_{l'})^2}{2} + U_n U^*_n \right]^{1/2} \tag{2.224}
$$

According to Eq. (216), close to the branch crossing point $q_m = \pi(l + l')/a$, the fraction participating in this result may be approximated as\(^{61}\)

\(^{60}\) Let me hope that the difference between this new integer and particle’s mass, both called $m$, is absolutely clear from the context.

\(^{61}\) Physically, $\beta \hbar = \hbar(n\pi/a)m = \hbar \tilde{E}^{(n)} / m$ is just the velocity of a free classical particle with energy $E^{(n)}$. 

\[
\frac{E_i - E_{i'}}{2} \approx \gamma \bar{q}, \quad \text{with} \quad \gamma \equiv \frac{dE_i}{dq} \bigg|_{q=q_m} = \frac{\pi \hbar^2 n}{ma} = \frac{2aE^{(n)}}{\pi n}, \quad \text{and} \quad \bar{q} \equiv q - q_m, \quad (2.225)
\]

while parameters \( E_{\text{ave}} \equiv (E_i + E_{i'})/2 = E^{(n)} \) and \( U_n U_n^* = |U_n|^2 \) do not depend on \( \bar{q} \), i.e. the distance from the central point \( q_m \). This is why Eq. (224) may be plotted as the famous level anticrossing (also called “avoided crossing”, or intended crossing”, or “non-crossing”) diagram (Fig. 29), with the energy gap width \( \Delta n \) equal to \( 2 |U_n| \), i.e. just double the magnitude of the \( n \)-th Fourier harmonic of the periodic potential \( U(x) \). Such anticrossings are also clearly visible in Fig. 28 that shows the results of the exact solution of Eq. (198) for \( \beta = 0.5 \).62

![Fig. 2.29. Level anticrossing diagram.](image)

We will run into the anticrossing diagram again and again in the course, notably at the discussion of spin. Such diagram characterizes any quantum systems with two weakly-interacting eigenstates with close energies. It is also repeatedly met in classical mechanics, for example at the calculation of eigenfrequencies of coupled oscillators.63,64 In our current case of the weak potential limit, the diagram describes the weak interaction of two sinusoidal de Broglie waves (216), with oppositely directed wave vectors, \( l \) and \( -l' \), via the \((l - l')^\text{th}\) (i.e. \( n^\text{th}\)) Fourier harmonic of the potential profile \( U(x) \). This effect exists also for the classical wave theory, and is known as the Bragg reflection, describing, for example, the 1D case of the wave reflection by a crystal lattice (Fig. 1.5) in the limit of weak interaction between the incident particles and the lattice.

Returning for the last time to our initial result – the band structure for the delta-functional \( U(x) \) (Fig. 24), shown in Fig. 26, we may wonder how general it is, taking into account the peculiar properties of the delta-function approximation. A partial answer may be obtained from the band structure for two more realistic and relatively simple periodic functions \( U(x) \): the sinusoidal potential (Fig. 30a) and the rectangular Kronig-Penney potential shown in Fig. 30b.

For the sinusoidal potential (Fig. 30a), with \( U(x) = U_1 \cos(2\pi x/\alpha) \), the stationary Schrödinger equation (61) takes the form

---

62 From that figure, it is also clear that in the weak potential limit, width \( \Delta E_n \) of the \( n \)-th energy band is just \( E^{(n)} - E^{(n-1)} \) – see Eq. (221). Note that this is exactly the distance between adjacent energy levels of the simplest 1D quantum well of infinite depth – cf. Eq. (1.77).

63 See, e.g., CM Sec. 5.1 and in particular Fig. 5.2.

64 Actually, we could obtain this diagram earlier in this section, for the system of two weakly coupled quantum wells (Fig. 23), if we assumed the wells to be slightly dissimilar.
\[-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + U_1 \cos \frac{2\pi x}{a} \psi = E \psi. \tag{2.226}\]

By the introduction of dimensionless variables

\[\xi \equiv \frac{\pi x}{a}, \quad \alpha \equiv \frac{E}{E^{(1)}}, \quad 2\beta \equiv \frac{U_1}{E^{(1)}},\tag{2.227}\]

where \(E^{(1)}\) is defined by Eq. (221), Eq. (226) may be reduced to the canonical form of the well-known Mathieu equation\(^{65}\)

\[\frac{d^2 \psi}{d\xi^2} + (\alpha - 2\beta \cos 2\xi) \psi = 0. \tag{2.228}\]

---

Figure 31 shows the so-called characteristic curves of the Mathieu equation, i.e. the relations between parameters \(\alpha\) and \(\beta\), corresponding to the energy band edges separating them from the adjacent bands. (Such curves may be readily calculated numerically, for example, using Eqs. (215) with the band-edge values \(qa = 0\) and \(qa = \pi\).) In such “phase plane” plots, the detailed information about the energy dependence on the quasi-momentum is lost, but we already know from Fig. 26 that the dependence is not too eventful. The most remarkable feature of these plots is the fast (exponential) disappearance of the allowed energy bands at \(2\beta > \alpha\) (in Fig. 31, above the red dashed line), i.e. at \(E < U_1\). This may be readily explained by our tight-binding approximation result (206): as soon as the eigenenergy drops significantly below the potential maximum \(U_{\text{max}} = U_1\) (see Fig. 30a), quantum states in the adjacent potential wells are only connected by tunneling through the separating potential barriers, with exponentially small amplitudes \(\delta_n\) – see Eq. (204).

On the other hand, the characteristic curves below the dashed line, i.e. at \(2\beta < \alpha\), correspond to virtually free motion of the particle with energy \(E\) above \(U_{\text{max}} = U_1\). Naturally, in this region the energy bands rapidly expand while gaps virtually disappear. This could be expected from the weak potential limit analysis (see Fig. 28 and its discussion); however, based on that analysis one could expect that the

---

\(^{65}\) This equation, first studied in the 1860s by É. Mathieu in the context of a rather practical problem of vibrating elliptical drumheads (!), has many other important applications in physics and engineering, notably including the parametric excitation of oscillations – see, e.g., CM Sec. 4.5.
energy gaps $\Delta_n \approx 2 |U_n|$ would disappear more gradually. The fast decline of the gaps at $U_1 \to 0$ (i.e. $\beta \to 0$) in the Mathieu equation is an artifact of the sinusoidal potential $U(x)$, with no Fourier harmonics $U_n$ above the first one. (In order to calculate the correct asymptotic behavior $\Delta_n \propto \beta^n$ at $\beta \to 0$, one needs to go beyond the first approximation we have used in the weak potential limit analysis.)

If one wants to study the details of transition between the two limits in the 1D band theory without the artifacts of the delta-functional model shown in Fig. 24 (with infinite number of harmonics $U_n$ independent of $n$) and of the Mathieu equation (with all $U_n = 0$ for $n \neq \pm 1$), the standard way is to examine the Kronig-Penney potential shown in Fig. 30b. For this potential, the characteristic equation may be readily derived using our rectangular barrier analysis in Sec. 3. For the case $E < U_0$, the result is the following natural generalization of Eq. (166):

$$\cos qa = \cosh \kappa d \cos k(a - d) + \frac{1}{2} \left( \frac{\kappa}{k} - \frac{k}{\kappa} \right) \sinh \kappa d \sin k(a - d),$$  \hspace{1cm} (2.229)

where parameters $k$ and $\kappa$ are defined, as functions of $E$ and $U_0$, by Eqs. (62) and (65). In the opposite case $E > U_0$, one can use the same formula with the replacement (73). Plots $E(q)$, described by these formulas,$^{66}$ are very similar to those shown in Figs. 26b and 28 above. In order to see some difference, one needs to plot the characteristic curves $U_0(E)$. This may be done by taking $qa = 0$ and $qa = \pi$ (i.e. $\cos qa = \pm 1$) in Eq. (229), and solving the resulting transcendental equation for $U_0$ numerically. The curves are generally similar to those shown in Fig. 31, but, in accordance with Eq. (224), exhibit a more gradual decrease of energy gaps:

$$\Delta_n \to 2 |U_n| \propto \frac{U_0}{n}, \quad \text{at} \quad E \sim E^{(n)} >> U_0.$$  \hspace{1cm} (2.230)

To conclude this section, let me address the effect of periodic potential on the number of eigenstates in 1D systems of large but finite length $l >> a, k^{-1}$. Surprisingly, the Bloch theorem makes the analysis of this problem elementary, for arbitrary $U(x)$. Indeed, let us assume that $l$ is comprised of

$^{66}$ Such plots, for several particular values of parameters, may be found, for example, in Figs. 8.11-8.13 of E. Merzbacher’s textbook cited above.
an integer number of periods $a$, and its ends are described by the similar boundary conditions – both assumptions evidently inconsequential for $l >> a$ (such as a 1-cm-scale crystal with $\sim 10^8$ atoms along each direction). Then, according to Eq. (210), the boundary conditions impose, on the quasi-momentum $q$, exactly the same quantization condition as we had for $k$ for a free 1D motion. Hence, instead of Eq. (1.94) we can write

$$dN = \frac{l}{2\pi} dq,$$  \hspace{1cm} (2.231)

with the corresponding change of the summation rule:

$$\sum_q f(q) \rightarrow \frac{l}{2\pi} \int f(q) dq.$$  \hspace{1cm} (2.232)

Hence, the density of states in 1D $q$-space, $dN/dq = l/2\pi$, does not depend on the potential profile at all! Note, however, that the profile does affect the density of states on the energy axis, $dN/dE$. As an extreme example, on the bottom and at the top of each energy band we have $dE/dq \rightarrow 0$, and hence

$$\frac{dN}{dE} = \frac{dN}{dq} \frac{dq}{dE} = \frac{l}{2\pi} \left( \frac{dE}{dq} \right) \rightarrow \infty.$$  \hspace{1cm} (2.233)

This divergence (which survives in higher spatial dimensionalities as well) of the state density has important implications for the operation of several electron and optical devices, in particular semiconductor lasers.

### 2.8. Effective mass and the Bloch oscillations

The band structure of the energy spectrum has profound implications not only on the density of states, but also on the dynamics of particles in periodic potentials. In order to see that, let us consider the simplest case: motion of a wave packet consisting of Bloch functions (210), all in the same (say, $n^{th}$) energy band. Similarly to Eq. (27) for the a free particle, we can describe such a packet as

$$\Psi(x,t) = \int a_q u_q(x) e^{i[qx - \omega(q)t]} dq,$$  \hspace{1cm} (2.234)

where the $a$-periodic functions $u(x)$, defined by Eq. (208), are now indexed to emphasize their dependence on the quasi-momentum, and $\omega(q) \equiv \frac{E_n(q)}{\hbar}$ is the function of $q$ describing the shape of the corresponding energy band – see, e.g., Fig. 26b or Fig. 28. If the packet is narrow, i.e. the width $\delta q$ of the distribution $a_q$ is much smaller than all the characteristic scales of the dispersion relation $\omega(q)$, in particular $\pi/a$, we may simplify Eq. (234) exactly as we have done in Sec. 2 for a free particle, despite the presence of factors $u_q(x)$ under the integral. In the linear approximation of the Taylor expansion, we again get Eq. (32), but now with

$$v_{gr} = \frac{d\omega}{dq} \bigg|_{q=q_0}, \quad \text{and} \quad v_{ph} = \frac{\omega}{q} \bigg|_{q=q_0},$$  \hspace{1cm} (2.235)

---

$^67$ A generalization of this expression to the case of essential interband transitions is not difficult using the Heisenberg picture of quantum mechanics (which will be discussed in Chapter 4 of this course) - see, e.g., Sec. 55 in E. M. Lifshitz and L. P. Pitaevskii, *Statistical Physics, Part 2*, Pergamon, 1980.
where \( q_0 \) is the central point of the quasi-momentum distribution. Despite the formal similarity with Eq. (33) for the free particle, this result is much more eventful; for example, as evident from the dispersion relation’s topology (see Figs. 26b, 28), the group velocity vanishes not only at \( q = 0 \), but at all values of \( q \) that are multiples of \((\pi/a)\), at the bottom and on the top of each energy band. At these points, packet’s envelope does not move in either direction - though may keep spreading.\(^{68}\)

Even more fascinating phenomena take place if a particle in the periodic potential is the subject of an additional external force \( F(t) \). (For electrons in a crystal lattice, this may be, for example, the Lorentz force of the applied electric and/or magnetic field.) Let the force be relatively weak, so that product \( Fa \) (i.e. the scale of energy increment from the additional force per one lattice period) is much smaller than the relevant energy scales the dispersion relation \( E(q) \) – see Fig. 26b:

\[
Fa \ll \Delta E_n, \Delta_n.
\]  

(2.236)

This relation allows one to neglect the force-induced interband transitions, so that the wave packet (234) includes the Bloch eigenfunctions belonging to only one (initial) energy band at all times. For the time evolution of its center \( q_0 \), theory yields\(^{69}\) an extremely simple equation of motion

\[
\dot{q}_0 = \frac{1}{\hbar} F(t). 
\]  

(2.237)

This equation is physically very transparent: it is essentially the 2\textsuperscript{nd} Newton law for the time evolution of the quasi-momentum \( \hbar q \) under the effect of the additional force \( F(t) \) only, excluding the periodic force \(-\partial U(x)/\partial x \) of the background potential \( U(x) \). This is very natural, because \( \hbar q \) is essentially the particle’s momentum averaged over potential’s period, and the periodic force effect drops out at such an averaging.

Despite the simplicity of Eq. (237), the results of its solution may be highly nontrivial. First, let us use Eqs. (235) and (237) find the instant \textit{group acceleration} of the particle (i.e. the acceleration of its wave packet’s envelope):

\[
a_{gr} = \frac{d^2q_{0}}{dt^2} = \frac{d}{dt} \left( \frac{d\omega(q_0)}{dq_0} \right) = \frac{d\omega(q_0)}{dq_0} \frac{dq_0}{dt} = \frac{d\omega(q_0)}{dq_0} \frac{dq_0}{dt} = \frac{1}{\hbar} \frac{d^2\omega}{dq^2} \bigg|_{q=q_0} F(t).
\]  

(2.238)

This means that the second derivative of the dispersion relation plays the role of the effective reciprocal mass of the particle:

\[
m_{ef} = \frac{\hbar}{d^2\omega/dq^2} = \frac{\hbar^2}{d^2E/dq^2}. 
\]  

(2.239)

For the particular case of a free particle, described by Eq. (216), this expression is reduced to the original (and constant) mass \( m \), but generally the effective mass depends on the wave packet’s momentum. According to Eq. (239), at the bottom of any energy band, \( m_{ef} \) is always positive, but depends on the strength of particle’s interaction with the periodic potential. In particular, according to Eq. (206), in the tight binding limit, the effective mass is very large:

---

\(^{68}\) For a Gaussian packet, the spreading is described by Eq. (39), with the replacement \( k \to q \); it is curious that at the inflection points with \( d^2\omega/dq^2 = 0 \) (which are present in each energy band) the packet does not spread.

\(^{69}\) The proof of Eq. (237) is not difficult, but becomes more compact in the bra-ket formalism, to be discussed in Chapters 4 and 5. This is why I recommend the proof to the reader as an exercise after reading those two chapters.
\[
|m_{\text{eff}}|_{q=(\pi/a)n} = \frac{\hbar^2}{2\delta q_a^2} = \frac{m}{\pi^2 \delta_n} \gg m. \tag{2.240}
\]

On the contrary, in the weak potential limit, the effective mass is close to \(m\) at most points of each energy band, but at the edges of the (narrow) bandgaps it is much smaller. Indeed, expanding Eq. (224) in the Taylor series near point \(q = q_m\), we get
\[
E_{\pm}(E \approx E^{(n)}) \approx \pm |U_n| \pm \frac{1}{2 |U_n|} \left( \frac{dE}{dq} \right)^2_{q=q_m} \tilde{q}^2 = \pm |U_n| \pm \frac{\gamma^2}{2 |U_n|} \tilde{q}^2, \tag{2.241}
\]
where \(\gamma\) and \(\tilde{q}\) are defined by Eq. (225), so that
\[
|m_{\text{eff}}|_{q=q_m} = |U_n| \frac{\hbar^2}{\gamma^2} = m \frac{|U_n|}{2E^{(n)}} \ll m. \tag{2.242}
\]

The effective mass effects in real solids may be very significant. For example, the charge carriers in the ubiquitous field-effect transistors of silicon integrated circuits have \(m_{\text{eff}} \approx 0.19 \, m_e\) in the lowest normally-empty energy band (traditionally called the conduction band), and \(m_{\text{eff}} \approx 0.98 \, m_e\) in the lower, normally-filled valence band. In some semiconducting compounds the conduction-band electron mass may be even smaller - down to 0.0145 \(m_e\) in InSb!

However, the absolute value of the effective mass in not the most surprising effect. The more shocking corollary of Eq. (239) is that on the top of each energy band the effective mass is negative – please revisit Figs. 26, 28, and 29 again. This means that the particle (or more strictly its wave packet’s envelope) is accelerated in the direction opposite to the force. This is exactly what electronic engineers, working with electrons in semiconductors, call holes, characterizing them by positive mass and positive charge. If the particle does not leave a close vicinity of the energy band’s top (say, due to scattering effects), such flip of signs does not lead to an error, because the Lorentz force is proportional to electron’s charge (\(q = -e\)), so that particle’s acceleration \(a_{\text{gr}}\) is proportional to ratio \((q/m_{\text{eff}})\).\(^{70}\)

However, at some phenomena the usual image of a hole as a particle with \(q > 0\) and \(m_{\text{eff}} > 0\) is unacceptable. For example, let us form a narrow wave packet at the bottom of the lowest energy band,\(^{71}\) and then exert on it a constant force \(F > 0\) – say, due to a constant external electric field directed along axis \(x\). According to Eq. (237), this would lead to a linear growth of \(q_0\) in time, so that in the quasi-momentum space, the packet’s center would slide, with constant speed, along the \(q\) axis – see Fig. 32a. Close to the energy band bottom, this motion would correspond to a positive effective mass (possibly, somewhat larger than the genuine particle’s mass \(m\)), and hence be close to free particle’s acceleration. However, as soon as \(q_0\) has reached the inflection point, where \(d^2E_1/dq^2 = 0\), the effective mass, and hence acceleration (238) change signs to negative, i.e. the packet starts to slow down (in the direct space

\(^{70}\) The language is which the hole has a positive charge and mass has an additional convenience for states on the top of the valence band whose single-particle states are normally filled. Then the simplest, single-particle excitation of this multi-particle ground state may be created by giving one electron enough energy to lift it to a reference (e.g., Fermi-energy) level \(E_F\) that is, by definition of the valence band, is higher than all values \(E(q)\). Then it is natural to prescribe to the excitation a positive mass \(m_{\text{eff}}\), because the energy \(\Delta E = E_F - E(q)\) necessary for the excitation grows with the deviation of \(q\) from \(q_m\).

\(^{71}\) Intuition tells us (and statistical physics duly confirms :-) that this may be readily done, for example, by weakly coupling the system to a low-temperature environment, and letting it to relax to the lowest possible energy.
\( x \) while still moving ahead in the quasi-momentum space. Finally, at the energy band’s top the particle stops at certain \( x_{\text{max}} \), while continuing to move in the \( q \)-space.

Now we have two alternative ways to look at the further time evolution of the wave packet. From the extended zone picture (which is the simplest for this analysis, see Fig. 32a),\(^{72}\) we may say that the particle crosses the 1st Brillouin zone boundary and starts going forward in \( q \), i.e. down the lowest energy band. According to Eq. (235), this region (up to the next inflection point) corresponds to a negative group velocity. After \( q_0 \) has reached the next minimum of the energy band at \( qa = 2\pi \), the whole process repeats again (and again, and again).

These are the famous Bloch oscillations – the effect that was predicted (by the same F. Bloch) as early as in 1929, but evaded experimental observation until the 1980s - see below. Their time period may be readily found from Eq. (237):

\[
\Delta t_B = \frac{\Delta q}{dq/dt} = \frac{2\pi/a}{F/h} = \frac{2\pi \hbar}{Fa},
\]

so that the Bloch oscillation frequency

\[
\omega_B = \frac{2\pi}{\Delta t_B} = \frac{Fa}{\hbar}.
\]

The direct-space motion of the wave packet’s center \( x_0(t) \) during the Bloch oscillation process may be analyzed by integrating Eq. (235) over some time interval \( \Delta t \):

---

\(^{72}\) This phenomenon may be also discussed from the point of view of the reduced zone picture, but then it requires the introduction of instant jumps between the Brillouin zone boundary points (see the dashed red line in Fig. 32) that correspond to physically equivalent states of the particle. Evidently, this language is more artificial.
\[
\Delta x_0(t) = \int_0^{\Delta t} N \sqrt{\frac{\hbar}{M}} dt = \int_0^{\Delta t} \frac{d\omega(q_0)}{dq_0} dq_0 = \frac{\hbar}{F} \int_{\omega=0}^{\omega=N} \frac{d\omega}{\omega} \Delta \omega(q_0).
\] (2.245)

If interval \(\Delta t\) is equal to the Bloch oscillation period \(\Delta t_B\) (234), the initial and final moments of \(E(q_0) = \hbar \omega(q_0)\) are equal, giving \(\Delta x_0 = 0\): in the end of the period, the wave packet returns to its initial position. However, if we carry this integration only from the smallest to the largest values of \(\omega(q_0)\), i.e. the points where the group velocity vanishes, we get the oscillation swing

\[
\Delta x_{\text{max}} = \frac{\hbar}{F} (\omega_{\text{max}} - \omega_{\text{min}}) = \frac{\Delta E_1}{F}.
\] (2.246)

This simple result may interpreted using an alternative energy diagram (Fig. 32b) that results from the following arguments. The additional force \(F\) may be described not only via the 2nd Newton law version (237), but, alternatively, by its contribution \(U_F = -Fx\) to the total (“Gibbs”\(^73\)) potential energy

\[
U_F(x) = U(x) + Fx
\] (2.247)
of the system. The direct solution of the Schrödinger equation (61) with such potential may be hard to find, but if the force is weak in the sense of Eq. (236), as we are assuming now, one can argue that our quantum-mechanical treatment including the periodic potential \(U(x)\) should be still correct, if the second term in Eq. (247) is considered as a constant at the wave packet width scale \(\delta x\), but dependent on position \(x_0\) of the packet’s center. In this approximation, the total energy of the wave packet may be found as

\[
E_x = E(q_0) - Fx_0.
\] (2.248)

In a plot of such energy as a function of \(x_0\) (Fig. 32b), the information on energy dependence on \(q_0\) is lost, but we already know it is rather uneventful, and well characterized by the position of band-gap edges on the energy axis.\(^74\) In this representation, the Bloch oscillations of a relatively wide \((\delta x >> a)\) wave packet should keep the full energy \(E_x\) constant, i.e. follow a horizontal line in Fig. 32b, limited by the classical turning points corresponding to the bottom and the top of the allowed energy band. The distance \(\Delta x_{\text{max}}\) between these point is evidently given by Eq. (246).

Besides this second look at the oscillation swing result, the total energy diagram shown in Fig. 32b enables one more remarkable result. Let a wave packet be so narrow in the momentum space \((\delta q \rightarrow 0)\) that \(1/q >> \Delta x_{\text{max}}\); then the horizontal line segment in Fig. 32b presents the spatial extension of the eigenfunction of the Schrödinger equation with potential (247). But this equation is evidently invariant with respect to the following simultaneous translation in coordinate and energy:

\[
x \rightarrow x + a, \quad E \rightarrow E - Fa.
\] (2.249)

This means that it is satisfied with an infinite set of similar solutions, each corresponding to one of the horizontal red lines shown in Fig. 32b. This is the famous Wannier-Stark ladder, with the step height

\[
\Delta E_S = Fa.
\] (2.250)

\(^73\) See, e.g., CM Sec. 1.5.

\(^74\) In semiconductor device physics and engineering, such plots are called the band edge diagrams, and are the virtually unavoidable components of any discussion or publication.
The importance of this alternative representation of the Bloch oscillations is due to the following fact. In most experimental realizations, the power of radiation at frequency (244), that may be extracted from the oscillations by their electromagnetic coupling to an external detector, is very low, so that their direct detection presents a hard problem. However, let us apply to a Bloch oscillator an additional rf field at frequency \( \omega \approx \omega_B \). As these frequencies are brought close together, the external signal should synchronize (“phase lock”) Bloch oscillations, resulting in certain observable changes – for example, a resonant absorption of the external radiation. Now let us notice that Eqs. (244) and (250) yield the following remarkable relation:

\[
\Delta E_s = h \omega_B. \tag{2.251}
\]

This means that the resonant phenomena at \( \omega \approx \omega_B \) allow for an alternative (but equivalent) interpretation – as the result of rf-induced transitions between the steps of the Wannier-Stark ladder! (Such occasions when two very different languages may be used for the interpretation of the same phenomenon is one of the most beautiful features of physics.)

This effect has been used for the first experimental confirmation of the Bloch oscillation theory. For this purpose, the natural periodic structures, solid state crystals, are inconvenient due to their very small period \( a \sim 10^{-10} \text{ m} \). Indeed, according to Eq. (244), such structures require very high forces \( F \) (and hence high electric fields \( E \equiv F/e \)) to bring \( \omega_B \) to an experimentally convenient range. This problem has been overcome by fabricating artificial periodic structures (superlattices) of certain semiconductor compounds, such as Ga\(_{1-x}\)Al\(_x\)As with various degrees \( x \) of gallium to aluminum atom replacement, whose layers may be grown over each other epitaxially, i.e., without very few crystal structure violations. These superlattices, with periods \( a \sim 10 \text{ nm} \), has allowed a clear observation of resonant effects at \( \omega \approx \omega_B \), and hence the measurement of the Bloch oscillation frequency, in particular its proportionality to the applied dc electric field, predicted by Eq. (244).78

Very soon after this observation, the Bloch oscillations have been observed in small Josephson junctions. Since this experiment involved two important conceptual issues, let me discuss it in a little bit more detail. As was discussed in Sec. 2.3, the Josephson junction dynamics may be reasonably well described by two simple equations (54) and (55). They may be combined to calculate the work of an external voltage source at Josephson phase change between arbitrary initial (\( \phi_{ini} \)) and final (\( \phi_{fin} \)) values, as the integral of its power \( IV \) over the time interval \( \Delta t \) of the change:

\[
\text{work} = \int_{\Delta t} IV dt = \int_{\Delta t} \left( I_c \sin \phi \frac{\hbar}{2e} \frac{d\phi}{dt} \right) dt = \frac{\hbar I_c}{2e} \int_{\phi_{ini}}^{\phi_{fin}} \sin \phi d\phi = -\frac{\hbar I_c}{2e} \left( \cos \phi_{fin} - \cos \phi_{ini} \right). \tag{2.252}
\]

We see that the work depends only on the initial and final values of \( \phi \) (but not on the law phase evolution in time), i.e. may be presented as the difference \( U(\phi_{fin}) - U(\phi_{ini}) \), where function

75 In systems with many independent particles (such as semiconductors), the detection problem is exacerbated by phase incoherence of the Bloch oscillations performed by each particle. This drawback is absent in atomic Bose-Einstein condensates whose Bloch oscillations (in a periodic potential created by standing optical waves) were eventually observed by M. Ben Dahan et al., Phys. Rev. Lett. 76, 4508 (1996).

76 A simple analysis of phase locking of a classical oscillator may be found, e.g., in CM Sec. 4.4.

77 A qualitative theory of such transitions will be discussed in Sec. 6.6 and then in Chapter 7.


may be interpreted as the potential energy of the junction (if we consider the Josephson phase as a
generalized coordinate). This energy apart, the Josephson junction, as a system of two close, nearly
isolated (super)conductors, has a certain capacitance $C$ and the associated electrostatic energy $E_C = CV^2/2$. Using Eq. (54) again, we may present it as

$$ E_C = \frac{C}{2} V^2 = C \left( \frac{\hbar}{2e} \right)^2 \left( \frac{d\varphi}{dt} \right)^2. $$

(2.251)

This means that from the point of view at phase $\varphi$ as a generalized coordinate, $E_C$ should be considered
the kinetic energy of the system, whose dependence on the generalized velocity $d\varphi/dt$ is similar to that
of a 1D mechanical particle, with an effective mass $m = C \left( \frac{\hbar}{2e} \right)^2$.

(2.252)

Hence the total energy of the junction, $E_C + U(\varphi)$, is formally similar to that of a 1D non-relativistic
particle in the sinusoidal potential with the $\varphi$-axis period $a_J = 2\pi$.

However, before using the results of the 1D band theory to this system, we have to resolve one
paradox (that was the subject of a lively discussion just about 30 years ago). When we develop the band
theory, we imply that its translation by period $a$ is (in principle) measurable, i.e. particle positions $x$ and
$(x + a)$ are distinguishable – otherwise Eq. (193) with $q \neq 0$ would not have much sense. For a
mechanical particle this assumption is very plausible, but less so for a Josephson junction. Indeed, for
example, if we change $\varphi$ by $a_J = 2\pi$ via changing the phase of one of superconductors, say $\varphi_1$ (Fig. 3)
by $2\pi$, then its wavefunction becomes $|\psi\rangle \exp\{i(\varphi_1 + 2\pi)\} = |\psi\rangle \exp\{i\varphi_1\}$, and it is not immediately
clear whether these two states may be distinguished. In order to resolve this contradiction, it is sufficient
to have a look at Eq. (54). It shows that if $\varphi$ changes in time by $2\pi$ (say, by a fast ramp-up), voltage $V$
across the junction exhibits a pulse with “area”

$$ \int V(t) \, dt = \frac{\hbar}{2e} \int \frac{d\varphi}{dt} \, dt = \frac{\hbar}{2e} \frac{\hbar}{2e} 2\pi = \frac{\hbar}{2e} \approx 2 \times 10^{-15} \text{ V} \cdot \text{s}. $$

(2.253)

Such single-flux-quantum (SFQ) pulses only not only may be measured experimentally, but even have been
used for signaling and ultrafast (sub-THz) computation, to the best of my knowledge still keeping the
absolute records for the highest speed and smallest energy consumption at computation.

Hence, the $2\pi$-shifts of phase $\varphi$ are measurable, and in the absence of dissipation the Josephson
junction dynamics is indeed similar to that of a 1D particle in a periodic (sinusoidal) potential, and its
energy spectrum forms energy bands and gaps described by the Mathieu equation – see Fig. 31.
Experimentally, the easiest way to verify this picture is to measure the corresponding Bloch oscillations

---

80 This unfortunate slip in the formula numbering can hardly lead to any misunderstanding.
81 Of course, the dimensionality of $m_{ef}$ so defined is different from kg.
82 This term has originated from the fact that the right-hand part of Eq. (253) equals to the single quantum unit
($\Phi_0$) of the magnetic flux in superconductors – see Sec. 3.1 below.
induced by an external current $I_{\text{ex}}(t)$. In order to find the frequency of these oscillations, it is sufficient to replace Eq. (237), which expresses the 2nd Newton law averaged over period $a$ of potential $U(x)$, with the charge balance equation

$$\frac{dQ}{dt} = I_{\text{ex}}(t), \quad (2.254)$$

where $Q$ is the “quasi-charge”\(^{84}\), i.e. the electric charge of the capacitor averaged over the period $2\pi$ of the periodic potential $U(\phi)$. (Notice that at such averaging, current (55) is averaged out from the equation, so that is affects the phenomena “only” via its contribution to the energy band structure.)

Since the Josephson-junction analog of the genuine wave number $k = m(dx/dt)/\hbar$ of a particle is

$$k = \frac{m_j}{\hbar} \frac{d\phi}{dt} = \frac{m_j}{\hbar} \frac{2e}{h} V = \frac{CV}{2e}, \quad (2.255)$$

and $CV$ is the genuine charge on the capacitor, the analog of $q$ (the quasi-momentum divided by $\hbar$) may be obtained just by the replacement of that product with quasi-charge $Q$:

$$q_j = \frac{Q}{2e}. \quad (2.256)$$

Comparing this expression with Eq. (254), we see that $q_j$ obeys the following equation of motion:

$$\frac{dq_j}{dt} = \frac{I_{\text{ex}}(t)}{2e}. \quad (2.257)$$

so that the role of force $F$ is now played by $F_j = hI/2e$. Hence if $I_{\text{ex}}(t) = \text{const} = \bar{I}$, we can use Eq. (244) with that replacement, and also $a \rightarrow a_j = 2\pi$, to get

$$f_B = \frac{\omega_n}{2\pi} = \frac{1}{2\pi} \frac{F_j a_j}{h} = \frac{\bar{I}}{2e}. \quad (2.258)$$

This very simple result has the following physical sense.\(^{85}\) In the quantum operation mode, the junction is recharged by the external current, following Eq. (256), until its electric charge reaches $e$ (i.e. $q_j a_j = (Q/2e)2\pi$ reaches $\pi$ - see Fig. 32a); then one Cooper pair passes through the junction changing its charge to $e - (2e) = -e$, with the same charging energy (251) – the process analogous to crossing the border of the 1st Brillouin zone; then the process repeats again and again. It is remarkable that Eq. (258), describing the frequency of such a quantum property of the Josephson phase $\phi$ as its Bloch oscillations, does not include the Planck constant, while Eq. (56), describing the classical motion of $\phi$, does.\(^{86}\)

---

\(^{84}\) Eq. (254) tells us that quasi-charge $Q$ has the simple physical sense of the external electric charge being inserted into the junction by the external current $I_{\text{ex}}$ - just like the physical sense of quasi-momentum $h\phi$ of a mechanical particle, according to Eq. (237), is the contribution to particle’s momentum by the external force $F$.


\(^{86}\) Phase locking of the Bloch oscillations, with frequency (258), as well as that of very similar SET oscillations of frequency $f_{\text{SET}} = I/e$, by a signal of well characterize frequency, enable fundamental standards of dc current. The experimentally achieved accuracy of such standards is close to $10^{-8}$, a few times worse than that of a less direct way - using the Josephson voltage standard and the resistance standard based on the quantum Hall effect.
In this context, one may wonder which of these two types of oscillations would a dc-biased Josephson junction generate. For the dissipation-free junction, the answer is: the Bloch oscillations (258) with frequency proportional to dc current. However, any practical junction has some energy losses that may be (approximately) described by a certain Ohmic conductance $G$ connected in parallel to the junction. Very luckily for Dr. Josephson and his Nobel Prize, it is much easier to fabricate and test junctions with $G >> 1/R_Q$, where $R_Q$ is the so-called quantum unit of resistance

$$R_Q \equiv \frac{\hbar}{2e^2} \approx 6.45 \text{k}\Omega,$$  \hspace{1cm} (2.259)

the fundamental constant that jumps out at analysis of several other effects as well – see, e.g., Sec. 3.2. As will be discussed in Chapter 7, such high energy losses provide what is called dephasing – the suppression of the quantum coherence between different quantum states of the system – in our current case, between the wavefunctions $u(\varphi - 2\pi j)$ localized at different minima of the periodic potential $U(\varphi)$, and thus make the dynamics of the Josephson phase $\varphi$ virtually classical, obeying equations (54) and (55). As we have seen in Sec. 2, dc biasing of such a junction leads to Josephson oscillations with frequency (56) proportional to the applied dc voltage.

### 2.9. Landau-Zener tunneling

All the Bloch oscillation discussion in the last section was based on the premise that the particle stays within one (say, the lowest) energy band. However, just a single look at Fig. 32 shows that this assumption becomes unrealistic if the energy gap separating this band from the next one becomes very small, $\Delta_1 \rightarrow 0$. Indeed, in the weak potential approximation, that is adequate in this limit, at $|U_1| \rightarrow 0$, the two dispersion curve branches (216) cross without any interaction, so that if our particle (the wave packet) is driven to approach that point, it should continue to move up in energy - see the dashed blue arrow in Fig. 32a. Similarly, in the “energy-domain” presentation shown in Fig. 32b, it is intuitively clear that at $\Delta_1 \rightarrow 0$, the particle residing at one of the steps of the Wannier-Stark ladder should able to somehow overcome the vanishing spatial gap $\Delta x_0 = \Delta_1/F$ and to leak into the next band – see the horizontal dashed blue arrow on that panel.

This process, called the Landau-Zener (or “interband”, or “band-to-band”) tunneling is indeed possible. In order to analyze it, let us first take $F = 0$, and consider what happens if a quantum particle described by an $x$-long (i.e. $E$-narrow) wave packet is incident from the free space upon a periodic structure of a large but finite length $l >> a$. If packet’s energy $E$ is within one of the energy bands, it may evidently propagate through the structure (though may be partly reflected from its front end). The corresponding quasi-momentum may be found by solving the dispersion relation for $q$: for example, in the weak-potential limit, Eq. (224), which is valid near the gap, yields

$$q = q_m + \bar{q}, \quad \bar{q} = \pm \frac{1}{\gamma} \left[ \frac{E^2}{\gamma} - \left|U_n\right|^2 \right]^{1/2}, \quad \text{where} \quad \bar{E} \equiv E - E^{(n)},$$  \hspace{1cm} (2.260)

and $\gamma$ is given by the second of Eqs. (225).

---

Now, if energy $E$ corresponds to one of the energy gaps $\Delta_n$, the propagation is impossible, so that the packet is completely reflected back. However, our analysis of the potential step problem in Sec. 3 implies that the wavefunction would still have an exponential tail protruding into the periodic structure and decaying on some length $\delta$ - see Eq. (67). Indeed, a review of the calculation leading to Eq. (260) shows that they remain valid within the gap as well, if the quasi-momentum is understood as a purely imaginary number:

$$q \to \pm i \kappa, \quad \text{where} \quad \kappa = \frac{1}{\gamma} \left[ |U_n|^2 - \bar{E}^2 \right]^{1/2}, \quad \text{for} \quad \bar{E}^2 \leq |U_n|^2. \quad (2.261)$$

With such contribution, the Bloch solution (193b) indeed describes an exponential decay of the wavefunction at length $\delta = 1/\kappa$.

Now returning to the effects of weak force $F$ in the energy-domain approach, presented by Eq. (248) and illustrated in Fig. 32b, we may recast Eq. (261) as

$$\kappa \to \kappa(x) = \frac{1}{\gamma} \left[ |U_n|^2 - (F \bar{x})^2 \right]^{1/2}, \quad (2.262)$$

where $\bar{x}$ is particle’s (i.e. wave packet center’s) deviation from the mid-gap point. Thus the gap has created a potential barrier of a finite width $\Delta x_0 = 2 |U_n|/F$, through which the wave packet may tunnel with a finite probability. As we already know, in the WKB approximation (in our case requiring $\kappa \Delta x_0 \gg 1$) this probability is just the tunnel barrier’s transparency $T$, which may be calculated from Eq. (117):

$$-\ln T = \frac{2}{\gamma} \int_{\kappa(x)^2 > 0} \kappa(x) dx = \frac{2}{\gamma} \int_{-\bar{x}_c}^{\bar{x}_c} \left[ |U_n|^2 - (F \bar{x})^2 \right]^{1/2} d\bar{x} = \frac{2 |U_n|}{\gamma} \int_{0}^{1/2} (1 - \xi^2)^{1/2} d\xi. \quad (2.263)$$

where $\pm \bar{x}_c \equiv \pm \Delta x_0/2 = \pm |U_n|/F$ are the classical turning points. Working out this simple integral (which may be viewed upon as the quarter of the unit circle’s area, and hence equal to $\pi/4$), we get

$$T = \exp \left\{ - \frac{\pi |U_n|^2}{\gamma F} \right\}. \quad (2.264)$$

This famous result was obtained by Landau and Zener in a more complex way, whose advantage is a constructive proof that Eq. (264) is valid for arbitrary relation between $\gamma F$ and $|U_n|^2$, i.e. arbitrary $T$, while our simple derivation was limited to the WKB approximation, i.e. to $T << 1$.

Returning to Eq. (225) and (237), we can rewrite the product $\gamma F$ participating in Eq. (264) as

$$\gamma F = \frac{1}{2} \left[ \frac{d(E_i - E_{i'})}{dq_0} \right]_{E_i = E_{i'} = E_n} \hbar \frac{dq_0}{dt} = \frac{\hbar}{2} \left[ \frac{d(E_i - E_{i'})}{dt} \right]_{E_i = E_{i'} = E_n} = \frac{\hbar u}{2}, \quad (2.265)$$

where $u$ has the meaning of the “speed” of the energy level crossing in the absence of the gap. Hence, Eq. (264) may be presented in a form

\[88\text{ Note that Eq. (264) is still limited to the hyperbolic dispersion relation, i.e. (in the band theory) to the weak potential limit. In the opposite, tight-binding limit, the interband tunneling may be treated as an excitation of the upper band states by sinusoidal Bloch oscillations, and is completely suppressed at } \hbar \omega_B < \Delta. \]
that is more physically transparent.\textsuperscript{89} Indeed, the fraction \(2\left|U_n\right|/u = \Delta_n u\) gives the time scale \(\Delta t\) of energy’s crossing the gap region, and according to the Fourier transform, its reciprocal, \(\omega_{\text{max}} \sim 1/\Delta t\) gives the upper cutoff of frequencies involved in the Bloch oscillation process. Hence Eq. (2.266) means that

\[
-\ln T \approx \frac{\Delta_n}{\hbar \omega_{\text{max}}}. \tag{2.267}
\]

This formula allows us to interpret the Landau-Zener tunneling as for system’s excitation across the energy gap \(\Delta_n\), by the maximum energy quantum \(\hbar \omega_{\text{max}}\) available from the Bloch oscillation process.

The interband tunneling is an important ingredient of several physical phenomena and even some practical devices, for example the tunneling (or “Esaki”) diodes. This simple device is just a junction of two semiconductor electrodes, one of them is so strongly \(n\)-doped by electron donors that the additional electrons form a degenerate Fermi gas at the bottom of the conduction band. Similarly, the opposite electrode is \(p\)-doped so strongly that the Fermi level of electrons in the valence band is lowered below the band edge (Fig. 33).

At thermal equilibrium, and in the absence of external voltage bias, the Fermi levels self-align,\textsuperscript{90} leading to the build-up of the contact potential difference \(\phi/e\), with \(\phi\) somewhat larger than the energy bandgap \(\Delta\) - see Fig. 33a. This potential difference creates an internal electric field that tilts the energy bands (just as the external field did in Fig. 32b), and leads to the formation of the so-called deletion layer in which the Fermi level located is within the energy gap and hence there are no charge carriers ready to move. In usual \(p-n\) junctions, this layer is broad and prevents any current at applied voltages \(V\) lower than \(\sim \Delta/e\). In contrast, in a tunneling diode the depletion layer is so thin (below \(\sim 10\) nm) that the

---

\textsuperscript{89} In Chapter 6, Eq. (266) will be derived using a different method based on the Golden Rule of quantum mechanics.

\textsuperscript{90} See, e.g., SM Secs. 1.5 and 6.4.
interband tunneling is possible and provides a substantial Ohmic current at small applied voltages – see Fig. 33c.

However, at substantial positive bias, \( eV \sim \Delta/2 \), the conduction band become aligned with the middle of the gap in the \( p \)-doped electrode, and electrons cannot tunnel there. Similarly, these are no electrons in the \( n \)-doped semiconductor to tunnel into the available states just above the Fermi level in the \( p \)-doped electrode – see Fig. 33b. As a result, current drops significantly, to grow again only when \( eV \) exceeds \( \sim \Delta \) and allows the electron motion through the within each energy band. Thus the tunnel junction’s \( I-V \) curve has a part with negative differential resistance (\( dV/dI < 0 \)). This effect may be used for the amplification of analog signals, including self-excitation of electrical oscillators (i.e. rf signal generation),\(^91\) and signal swing restoration in digital electronics.

2.10. Harmonic oscillator: A brute force approach

To complete our review of 1D systems, we have to consider the famous harmonic oscillator, i.e. a 1D particle moving in the quadratic-parabolic potential (111). This is just a smooth quantum well providing “soft” confinement, whose discrete spectrum we have already found in the WKB approximation – see Eq. (114). Let us try to solve the same problem exactly – not because there is anything conceptually interesting in it (there is not :-), but because of its enormous importance for applications. For that, let us write the stationary Schrödinger equation for potential (111):

\[
-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \frac{m \omega_0^2}{2} x^2 \psi = E \psi .
\]  
(2.268)

From the solution of Exercise Problem 1.5, the reader already knows\(^92\) one of the eigenfunctions of this equation,

\[
\psi_0 = C_0 \exp \left\{- \frac{m \omega_0 x^2}{2\hbar} \right\},
\]  
(2.269)

and the corresponding eigenenergy

\[
E_0 = \frac{\hbar \omega_0}{2} .
\]  
(2.270)

Expression (269) shows that the characteristic scale of wavefunction’s spatial spread\(^93\) is equal to

\[
x_0 \equiv \left( \frac{\hbar}{m \omega_0} \right)^{1/2} .
\]  
(2.271)

Due to the importance of this scale, let us give its crude estimates for several typical systems:

\(^91\) See, e.g., CM Sec. 4.4.

\(^92\) If not yet, I am inviting him or her to check this fact now by the direct substitution of solution (269) into the differential equation (268), simultaneously proving Eq. (270).

\(^93\) Quantitatively, as was already mentioned in Sec. 2.1, \( x_0 = \sqrt{2} \delta x = (2\bar{x}^2)^{1/2} \).
(i) Electrons in solids and fluids: \( m \approx 10^{-30} \text{ kg}, \ \omega_0 \sim 10^{15} \text{ s}^{-1} \), giving \( x_0 \sim 0.3 \text{ nm} \), comparable with inter-atomic distances \( a \). As a result, classical mechanics is not valid at all for the analysis of their motion.

(ii) Atoms in solids: \( m \approx 10^{-24} - 10^{-26} \text{ kg}, \ \omega_0 \sim 10^{13} \text{ s}^{-1} \), giving \( x_0 \sim 0.01 - 0.1 \text{ nm} \), i.e. from ~a few percent to a few tens percent of \( a \). Because of that, methods based classical mechanics (e.g., molecular dynamics) are approximately valid for the analysis of atomic motion, though may miss some fine effects of motion of lighter atoms – e.g., quantum tunneling of hydrogen atoms through energy barriers of the potential profile created by its neighbors.

(iii) Probe masses in modern gravity-wave detectors (Advanced LIGO, VIRGO, KAGRA, etc.): \( m \sim 10^2 \text{ kg}, \ \omega_0 \sim 10^2 \text{ s}^{-1} \), giving \( x_0 \sim 10^{-19} \text{ m} \). After several decades of development, the sensitivity of these instruments is still limited by various noise sources at the level of the order of \( 10^{-18} \text{ m} \). Thus the prospects of observing quantum-mechanical effects in such installations do not look very realistic.

Returning to the Schrödinger equation (268), let us recast it into a dimensionless form by introducing dimensionless variable \( \xi \equiv x/x_0 \). This gives

\[
-\frac{d^2 \psi}{d\xi^2} + \xi^2 \psi = \varepsilon \psi ,
\]

(2.272)

where \( \varepsilon \equiv 2E/h\omega_0 = E/E_0 \). In this notation, the ground state wavefunction is proportional to \( \exp\{-\xi^2/2\} \), so that let us look for the solutions to Eq. (272) in the form

\[
\psi = C \exp\left\{-\frac{\xi^2}{2}\right\} H(\xi) ,
\]

(2.273)

where \( H(\xi) \) is a new function. With this substitution, Eq. (272) yields

\[
\frac{d^2 H}{d\xi^2} - 2\xi \frac{dH}{d\xi} + (\varepsilon - 1)H = 0 .
\]

(2.274)

It is evident that \( H = \text{const} \) and \( \varepsilon = 1 \) is one of its solutions, describing the eigenstate (269) with energy (270), but what are the other eigenstates and eigenvalues? This equation has been studied in detail in the mid-1800s by C. Hermite who has shown that all eigenvalues are given by equation

\[
\varepsilon_n - 1 = 2n, \quad \text{with} \quad n = 0, 1, 2, \ldots,
\]

(2.275)

so that our WKB result (114) is indeed exact for any \( n \), and Eqs. (269) and (270) describe the ground-state of the oscillator. The eigenfunction corresponding to eigenvalue \( \varepsilon_n \) is a polynomial (now called the Hermite polynomial) of degree \( n \), that may be most conveniently calculated using the following explicit formula:

\[
H_n = (-1)^n \exp\left\{\frac{\xi^2}{2}\right\} \frac{d^n}{d\xi^n} \exp\{-\xi^2\} .
\]

(2.276)

---


95 According to the recent announcement by B. Abbott et al., Phys. Rev. Lett. 116, 061102 (2016), this sensitivity was sufficient for the first direct detection of gravitational waves emitted at a merger of two black holes.
It is easy to use this formula to calculate several lowest-degree polynomials – see Fig. 34a:

\[ H_0 = 1, \quad H_1 = 2\xi, \quad H_2 = 4\xi^2 - 2, \quad H_3 = 8\xi^3 - 12\xi, \quad H_4 = 16\xi^4 - 48\xi^2 + 12, \ldots \]  \hspace{1cm} (2.277)

The most important properties of the polynomials are as follows:

(i) their “parity” (symmetry-antisymmetry) alternates with number \( n \),

(ii) \( H_n(\xi) \) crosses the \( \xi \)-axis exactly \( n \) times (has \( n \) zeros), and

(iii) the polynomials are mutually orthonormal in the following sense:

\[
\int_{-\infty}^{+\infty} H_n(\xi) H_m(\xi) \exp\left\{-\xi^2\right\} d\xi = \pi^{1/2} 2^n n! \delta_{n,m}.
\]  \hspace{1cm} (2.278)

Fig. 2.34. (a) A few lowest Hermite polynomials and (b) the corresponding eigenenergies (dashed lines) and eigenfunctions (solid lines) of the harmonic oscillator. The black dashed line shows the potential profile \( U(x) \), drawn on the same scale as energies \( E_n \), so that the line crossings with the energy levels correspond to the classical turning points.
Using Eq. (273) to translate this result to functions $\psi_n(x)$, we get the following orthonormal eigenfunctions of the harmonic oscillator (Fig. 34b):\(^\text{96}\)

$$\psi_n(x) = \frac{1}{(2^n n!)^{1/2} \pi^{1/4} x_0^{1/2}} \exp \left\{ -\frac{x^2}{2x_0^2} \right\} H_n \left( \frac{x}{x_0} \right).$$ \hspace{1cm} (2.279)

Besides its own importance, this is a typical example of eigenstates of particle confined in a soft-wall quantum well. It is very instructive to compare them with eigenstates of a the rectangular quantum well, with its ultimately-hard walls – see Eq. (1.76) and Fig. 1.7. Let us list their similar features:

(i) Wavefunctions oscillate in the classically-allowed regions with $E_n > U(x)$, while dropping exponentially beyond the boundaries of that region.

(ii) Each step up the energy level ladder increases the number of the oscillation half-waves (and hence the number of its zeros), by one.\(^\text{97}\)

Here are the major features specific for the soft confinement:

(i) The spatial spread of the wavefunction grows with $n$, following the gradual increase of the classically allowed region.

(ii) Correspondingly, $E_n$ exhibits a slower growth than the $E_n \propto n^2$ law given by Eq. (1.77), because of the gradual reduction of confinement, which moderates the growth of kinetic energy.

Unfortunately, the brute-force approach to the harmonic oscillator problem, discussed above, is not too appealing intellectually. First, the proof of Eq. (276) is rather longish. More importantly, it is hard to use Eq. (279) for calculation of the so-called matrix elements of the system – as we will see in Chapter 4, virtually the only numbers important for applications. Finally, it is also almost evident that there should be some straightforward math leading to any formula as simple as Eq. (114) for $E_n$. Indeed, there is a much more efficient, operator-based approach to this problem; it will be described in Sec. 5.4.

### 2.11. Exercise problems

2.1. The initial wave packet of a free 1D particle is described by Eq. (2.20) of the lecture notes:

$$\Psi(x,0) = \int a_k e^{ikx} dk.$$  

(i) Obtain a compact expression for the expectation value $\langle p \rangle$ of particle's momentum. Does $\langle p \rangle$ depend on time?

(ii) Calculate $\langle p \rangle$ for the case when function $|a_k|^2$ is symmetric with respect to some value $k_0$.

2.2. Calculate the function $a_k$, defined by Eq. (2.20), for the wave packet with a rectangular envelope:

\(^{96}\) These stationary states of the harmonic oscillator are sometimes called its Fock states, to distinguish them from other fundamental solutions (such as Glauber states) which will be discussed in Sec. 5.5 and beyond.

\(^{97}\) In mathematics, a slightly more general statement, valid for a broader class of ordinary linear differential equations, is frequently called the Sturm oscillation theorem, and is a part of the Sturm-Liouville theory of such equations – see, e.g., Chapter 10 in the handbook by G. Arfken et al. recommended in MA Sec. 16.
\[ \Psi(x,0) = \begin{cases} C \exp[i k_0 x], & \text{for } -a/2 \leq x \leq +a/2, \\ 0, & \text{otherwise.} \end{cases} \]

Analyze the result in the limit \( k_0 a \to \infty. \)

2.3. Prove Eq. (49) for the 1D propagator of a free quantum particle, starting from Eq. (48).

2.4. Express the 1D propagator, defined by Eq. (44), via eigenfunctions and eigenenergies of a particle moving in an arbitrary stationary potential \( U(x). \) (For the notation simplicity, assume that the energy spectrum of the system is discrete.)

2.5. Calculate the change of the wavefunction of a 1D particle, resulting from a short pulse of an external force, which may be approximated by the delta-function:
\[ F(t) = P \delta(t). \]

2.6. Analyze the effect of phase locking of Josephson oscillations on the dc current flowing through the junction, assuming that external microwave source applies a fixed sinusoidal ac voltage,
\[ V(t) - \overline{V} = A \cos \omega t, \]

to a junction with sinusoidal current-phase relation (55), using Eq. (54) for time evolution of phase \( \varphi. \)

2.7. Calculate the transmission coefficient \( T \) as a function of particle’s energy \( E \) for the rectangular potential barrier,
\[ U(x) = \begin{cases} 0, & \text{for } x < -d/2, \\ U_0, & \text{for } -d/2 < x < +d/2, \\ 0, & \text{for } d/2 < x, \end{cases} \]

for the case \( E > U_0. \) Analyze and interpret the result, taking into account that \( U_0 \) may be either positive or negative. (In the last case, we are speaking about particle’s passage over a rectangular potential well of finite depth.)

2.8. Looking at the lower (red) line in Fig. 1.7, it seems plausible that the 1D ground-state function \( X(x) \propto \sin(\pi x/a) \) of the simple quantum well (1.69) may be well approximated by an inverted parabola:
\[ X_{\text{trial}}(x) = Cx(a-x), \]

where \( C \) is the normalization constant, and \( a \equiv a_0 \) for brevity. Explore how good this approximation is.

2.9. Spell out the stationary wavefunctions of a harmonic oscillator in the WKB approximation, and use them to calculate the expectation values \( \langle x^2 \rangle \) and \( \langle x^4 \rangle \) for arbitrary state number \( n. \)

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98 The constant \( P \) is called the force’s impulse. (In higher dimensionalities, it is a vector - just as the force is.)

99 Solving this problem is a good preparation to the use of the full variational method in the next two problems (and beyond).
2.10. A 1D particle of mass $m$ is placed into the following triangular quantum well:

$$U(x) = \begin{cases} +\infty, & \text{for } x < 0, \\ Fx, & \text{for } x > 0, \end{cases} \text{ with } F > 0.$$ 

(i) Calculate its energy spectrum using the WKB approximation.

(ii) Estimate the ground state energy using the variational method.

(iii) Calculate the three lowest energy levels, and also for the 10th level, with at least 0.1% accuracy, from the exact solution of the problem.

(iv) Compare and discuss the results.

Hints:

- In Task (ii), try to incorporate a certain parameter $\lambda$ into your trial wavefunction, and then use its adjustment to minimize the expectation value of system’s Hamiltonian (mentioned in Chapter 1):

$$\langle H \rangle_{\text{trial}} \equiv \frac{\int_{-\infty}^{+\infty} \psi_{\text{trial}}^* \hat{H} \psi_{\text{trial}} dx}{\int_{-\infty}^{+\infty} |\psi_{\text{trial}}|^2 dx},$$

where the trial function is assumed to be properly normalized. The variational method is based on the easily provable\(^{101}\) fact that this expectation value cannot be less than the genuine $E_g$, coinciding with it only if the trial function exactly coincides with the genuine wavefunction $\psi_g$ of the ground state. Hence, the lower $\langle H \rangle_{\text{trial}}$ you reach, the better is your result.

- The values of the first zeros of the Airy function, necessary for Task (iii), may be found in many math handbooks, for example, in Table 10.13 of the collection edited by Abramowitz and Stegun – see MA Sec. 16(i).

2.11. For a 1D particle of mass $m$ placed into a potential well with the following profile,

$$U(x) = ax^{2s}, \text{ with } a > 0 \text{ and } s > 0,$$

(i) calculate its energy spectrum using the WKB approximation, and

(ii) estimate the ground state energy using the variational method.

Compare the ground state energy results for parameter $s$ equal to 1, 2, 3, and 100.

2.12. Prove Eq. (117) for the case $T_{\text{WKB}} \ll 1$, using the connection formulas (104).

2.13. Use the WKB approximation to express the expectation value of the kinetic energy of a 1D particle, confined in a soft potential well, in its $n^{\text{th}}$ stationary state, via the derivative $dE_n/dn$, for $n \gg 1$.

2.14. Use the WKB approximation to calculate the transparency $T$ as a function of particle energy $E$, for the following triangular potential barrier:

$$U(x) = \begin{cases} 0, & \text{for } x < 0, \\ U_0 - Fx, & \text{for } x > 0, \end{cases}$$

\(^{100}\) With $F = mg$, this is just the well-known bouncing ball problem.

\(^{101}\) See, e.g., Sec. 8.2 below.
with \( F, U_0 > 0 \).

*Hint:* Be careful treating the sharp potential step at \( x = 0 \).

2.15. Prove that the symmetry of the scattering matrix elements describing an arbitrary time-independent scatterer allows its representation in the form (136a), with the additional restriction (136b).

2.16. Prove the universal relations between elements of the transfer matrix \( T \) of a stationary (but otherwise arbitrary) 1D scatterer, which were mentioned in Sec. 5.

2.17. For a deep and narrow 1D quantum well, modeled by a delta-function,

\[
U(x) = -\omega \delta(x), \quad \text{with } \omega > 0, \tag{*}
\]

find the localized eigenfunction(s) \( \psi_n \) (with \( |\psi_n(x)| \to 0 \) at \( |x| \to \infty \)), and the corresponding value(s) \( E_n \).

2.18. A 1D particle was localized in the delta-functional well, with \( U(x) = -\omega \delta(x) \), such as the one analyzed in the previous problem. Then (say, at \( t = 0 \)) the well’s bottom is suddenly lifted, so that the particle becomes free to move. Calculate the probability density, \( w(k) \) to find the particle in a state with wave number \( k \) at \( t > 0 \), and the final total energy of the system.

2.19. Calculate the lifetime of the metastable localized state of a 1D particle in the potential

\[
U(x) = -\omega \delta(x) - Fx, \quad \text{with } \omega > 0,
\]

using the WKB approximation. Formulate the condition of validity of the result.

2.20. Analyze the localized eigenfunction(s) and the characteristic equation(s) for eigenenergies of a 1D particle in the following two-well potential

\[
U(x) = -\omega \left[ \delta\left(x - \frac{a}{2}\right) + \delta\left(x + \frac{a}{2}\right) \right], \quad \text{with } \omega > 0.
\]

Explore asymptotic behaviors of the eigenenergies in the limits of very strong and very weak potential, and find the number of localized states as a function of distance \( a \).

2.21. * Consider a symmetric system of two quantum wells of the type shown in Fig. 23, but with \( U(0) = U(\pm \infty) = 0 \) – see Fig. on the right. What is the sign of well interaction force due to a quantum particle of mass \( m \), shared by them, for the cases when the particle is in:

(i) a symmetric eigenstate, with \( \psi_{\pm}(x) = \psi_{\pm}(x) \)?

(ii) an asymmetric eigenstate, with \( \psi_{\pm}(x) = -\psi_{\pm}(x) \)?

Use a different approach to confirm your result for the particular case of delta-functional wells, considered in the previous problem.

2.22. Derive and analyze the characteristic equation for eigenvalues for a particle in a rectangular well of a finite depth:
\[ U(x) = \begin{cases} -U_0, & \text{for } |x| \leq a/2, \\ 0, & \text{otherwise.} \end{cases} \]

In particular, calculate the number of localized states as a function of well’s width \( a \), and explore the limit \( U_0 \ll \hbar^2/2ma^2 \).

2.23. Calculate energy \( E \) of the localized state in a quantum well of an arbitrary shape \( U(x) \), provided that its width \( a \) is finite, and the average depth is very small:

\[ |U| \ll \frac{\hbar^2}{2ma^2}, \quad \text{where } U \equiv \frac{1}{a_{\text{well}}} \int U(x)dx. \]

2.24. A particle of mass \( m \) is moving in a field with the following potential:

\[ U(x) = U_0(x) + \omega \delta(x), \]

where \( U_0(x) \) describes a smooth, symmetric function with \( U_0(0) = 0 \), growing monotonically at \( x \to \pm \infty \).

(i) Use the WKB approximation to derive the characteristic equation for the energy spectrum;
(ii) semi-quantitatively describe the spectrum structure evolution at the increase of \( |\omega| \), for both signs of this parameter, and make the results more specific for the quadratic potential

\[ U_0(x) = \frac{m}{2} \omega_0^2 x^2. \]

2.25. Prove Eq. (191), starting from Eq. (190).

2.26. For the problem explored in the beginning of Sec. 7, i.e. 1D particle’s motion in a delta-functional periodic potential shown in Fig. 24,

\[ U(x) = \omega \sum_{j=-\infty}^{\infty} \delta(x - ja), \quad \text{with } \omega > 0, \]

(where \( j \) are integers), write explicit expressions for its eigenfunctions:

(i) at the bottom, and
(ii) at the top

of the lowest energy band. Sketch both eigenfunctions.

2.27. A 1D particle of mass \( m \) moves in an infinite periodic system of very narrow and deep quantum wells that may be described by delta-functions:

\[ U(x) = \omega \sum_{j=-\infty}^{\infty} \delta(x - ja), \quad \text{with } \omega < 0. \]

(i) Sketch the energy band structure of the system for relatively small and relatively large values of the quantum well’s “area” \( |\omega| \), and
(ii) calculate explicitly the ground state energy of the system in the limits of very small and very large \(|w|\).

2.28. For the system discussed in the previous problem, write explicit expressions for the eigenfunctions of the system, corresponding to:

(i) the bottom points of the lowest energy band, and
(ii) the top points of that band, and
(iii) the lowest points of each higher energy band,

and sketch the functions.

2.29. The 1D “crystal”, analyzed in the last two problems, now extends along only to \(x > 0\), while bordering a flat potential step at \(x = 0\):

\[
U(x) = \begin{cases} 
\sum_{j=1}^{\infty} \delta(x - ja), & \text{with } w < 0, \\
U_0 > 0, & \text{for } x < 0.
\end{cases}
\]

Prove that the system can have a set of so-called Tamm states, localized near the “surface” \(x = 0\), and calculate their energies in the limit when \(U_0\) is very large but finite. (Quantify this condition.)

2.30. Calculate the whole transfer matrix of the rectangular tunnel barrier, specified by Eq. (76), for particle energies both below and above \(U_0\).

2.31. Use results of the previous problem to calculate the transfer matrix of one period of the periodic Kronig-Penney potential shown in Fig. 30b (reproduced in Fig. on the right).

2.32. Using results of the previous problem, derive the characteristic equations for particle’s motion in the periodic Kronig-Penney potential, for both \(E < U_0\) and \(E > U_0\). Try to bring the equations to a form similar to that obtained in Sec. 5 for the delta-functional barriers – see Eq. (166). Use the equations to formulate the conditions of applicability of the tight-binding and weak-potential approximations, in terms of parameters \(U_0\), \(d\), and \(a\) of the potential profile, and particle’s mass \(m\) and energy \(E\).

2.33. For the Kronig-Penney potential, use the tight binding approximation to calculate the widths of the allowed energy bands. Compare the results with those of the previous problem (in the corresponding limit).

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102 In applications to electrons in solid-state crystals, the delta-functional quantum wells model the attractive potential of atomic nuclei, while \(U_0\) represents the workfunction, i.e. the energy necessary for the extraction of an electron from the crystal to the free space – see, e.g., EM Sec. 2.6 and SM Sec. 6.4.
2.34. For the same Kronig-Penney potential, use the weak potential limit formulas to calculate the energy gap widths. Again, compare the results with those of Problem 30, in the corresponding limit.

2.35. 1D periodic chains of atoms may exhibit what is called the so-called Peierls instability, leading to the Peierls transition to phase in which atoms are slightly displaced by \( \Delta x_j = (-1)^j \Delta x \), with \( \Delta x \ll a \). These displacements lead to the alternation of coupling amplitudes \( \delta_n \) (see Eq. (204)) between some values \( \delta_n^+ \) and \( \delta_n^- \). Use the tight-binding approximation to calculate the resulting change of the \( n \)th energy band, and discuss the result.

2.36. Assuming the quantum effects to be small, calculate the lower part of the energy spectrum of the following system: a small bead of mass \( m \), free to move without friction along a ring of radius \( R \) that is rotated about its vertical diameter with a constant angular velocity \( \omega \) - see Fig. on the right.\(^ {103} \) Formulate a quantitative condition of validity of your results.

2.37. A 1D harmonic oscillator (with mass \( m \) and frequency \( \omega_0 \)) had been in its ground state; then an additional force \( F \) was suddenly applied (and retained constant in time). Find the probability of the oscillator staying in its ground state.

2.38. A 1D particle of mass \( m \) has been placed into a quadratic potential well (111),

\[
U(x) = \frac{m\omega_0^2}{2} x^2,
\]

and allowed to relax into the ground state. Harmonic oscillator had been in its ground state. At \( t = 0 \), the well starts to be moved with velocity \( v \), without changing its profile, so that at \( t \geq 0 \) the above formula for \( U \) is valid with the replacement \( x \rightarrow x' = x - vt \). Calculate the probability for the system to still be in the ground state at \( t > 0 \).

2.39. A 1D particle is placed into the following potential well:

\[
U(x) = \begin{cases} 
+\infty, & \text{for } x < 0, \\
\frac{m\omega_0^2}{2} x^2, & \text{for } x \geq 0.
\end{cases}
\]

(i) Find its eigenstates and eigenenergies.

(ii) This system had been let to relax into its ground state, and then the potential wall at \( x < 0 \) was rapidly removed, so that the system was instantly turned into the usual harmonic oscillator (with the same \( m \) and \( \omega_0 \)). Find the probability for the oscillator to be in its ground state.

2.40. Prove the following formula for the propagator of the 1D harmonic oscillator:

\(^{103} \) This system was used as the analytical mechanics “testbed problem” in the CM part of this series, and the reader is welcome to use any relations derived there - but remember that they pertain to the classical mechanics domain!
\[ G(x,t;x_o,t_o) = \left( \frac{m\omega_0}{2\pi\hbar \sin[\omega_0(t-t_o)]} \right)^{1/2} \exp \left\{ \frac{i m\omega_0}{2\hbar \sin[\omega_0(t-t_o)]} \left[ (x^2 + x_o^2) \cos[\omega_0(t-t_o)] - 2xx_o \right] \right\}. \]

Discuss the relation between this formula and the propagator of a free 1D particle.

2.41. Use the variational method to estimate the ground state energy \( E_g \) of the following confined 1D systems:

(i) a harmonic oscillator, with \( U(x) = \frac{m\omega_0^2}{2} x^2 / 2 \), and

(ii) a particle in the following potential well: \( U(x) = -U_0 \exp \{-\alpha^2 x^2 \} \), and \( U_0 > 0 \).

In the latter case, get explicit results in the limits of small and large \( U_0 \), and give their interpretation.

2.42. * Use the WKB approximation to calculate the lifetime of the metastable ground state of a 1D particle of mass \( m \) in the “pocket” of the potential profile

\[ U(x) = \frac{m\omega_0^2}{2} x^2 - \alpha x^3. \]

Contemplate the significance of this problem.

2.43. In the context of the Sturm oscillation theorem mentioned in Sec. 10, prove that the number of zeros of stationary wavefunctions of a particle, confined in an arbitrary potential well, always increases with energy.

*Hint:* You may like to use the suitably modified Eq. (189).